Theories, Results, and Databases of Topology in Materials

https://www.topologicalquantumchemistry.com
https://www.topologicalquantumchemistry.fr/magnetic/
https://www.topologicalquantumchemistry.com/mltqc/
https://www.cryst.ehu.es/

U.S. DEPARTMENT OF ENERGY

SIMONS FOUNDATION

NSF

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Collaborators

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https://www.cryst.ehu.es/

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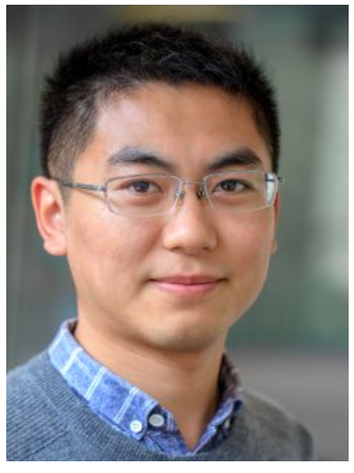

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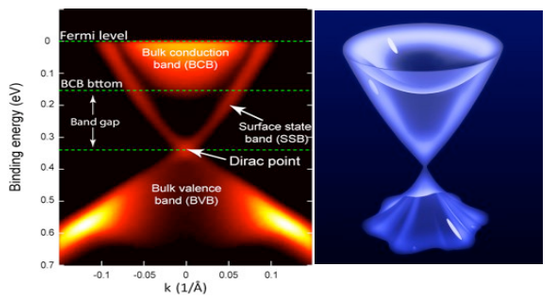
Outline

https://www.topologicalquantumchemistry.com
https://www.topologicalquantumchemistry.fr/magnetic/
https://www.topologicalquantumchemistry.com/mltqc/
https://www.cryst.ehu.es/

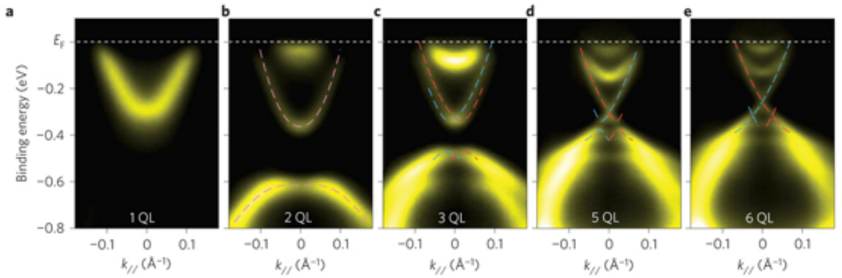
- Background: Topological Quantum Chemistry
- Theory: Magnetic Topological Quantum Chemistry (MTQC)
- Calculation methods
- Results: Topological phase diagrams and High-Throughput Topology
- Magnetic and NonMagnetic Material Database
- Ideal topological materials and new systems
- Topology from machine learning
- Future Directions

Discovery of topological materials



Hsieh Nature (2008)
Zhang Nat Phys (2009)
Xia Nat Phys (2008)

3D TIs theory + experiment : Bi_2Se_3

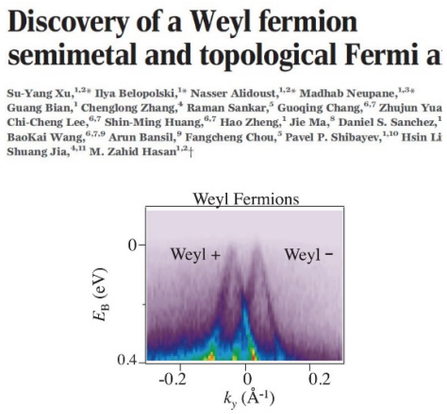


Chang Science (2013)

QAHE

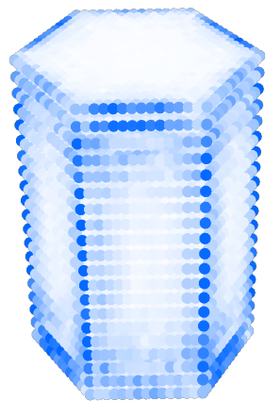
Weng PRX (2015)
Xu Science (2015)

Weyl semimetals



Bradlyn (2016)

New Fermions



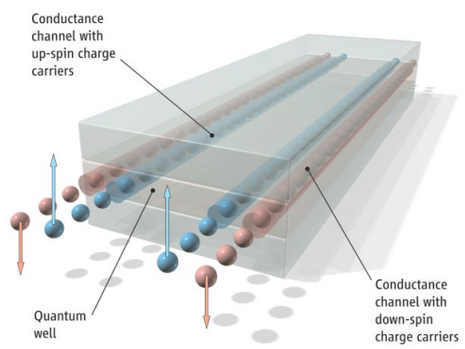
Nodal Lines

Bzdušek (2016)

2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018

Prediction HgTe 2D TI

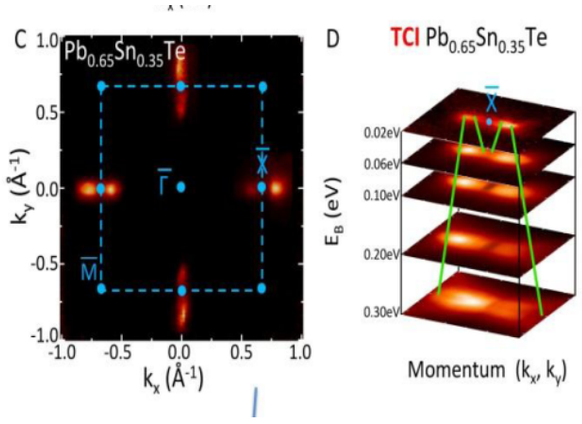
Bernevig Science (2006)
König Science (2007)



Kane & Mele, PRL (2015)

Mirror Chern insulators

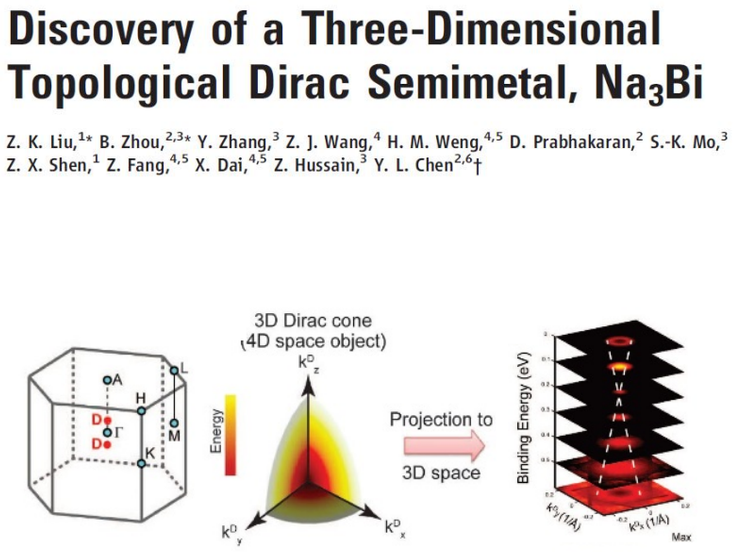
Hsieh Nat Comm (2012)
Tanaka Nat Phys (2012)



Type II Weyls

Soluyanov (2015)

Dirac semimetals

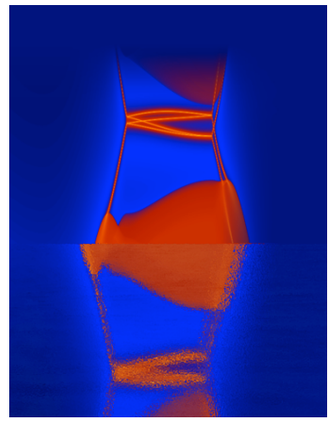


Non-symmorphic TIs

Alexandrinata (2016)

High Order TIs

Schindler (2018)



Topological Quantum Chemistry
Machine Learning

➡ Space group: set of symmetries for a 3D crystal structure

230 Space-Groups

- unit lattice translations ($\mathbf{Z}^3$)
- point group operations (rotations, reflections)
- non-symmorphic (screw, glide)
- orbitals
- atoms in some lattice positions

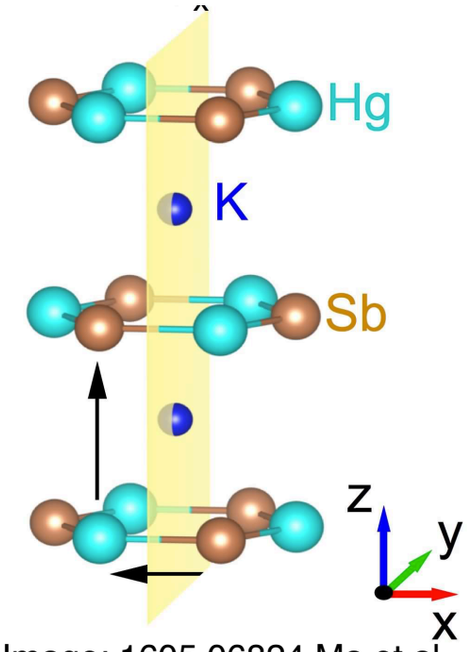


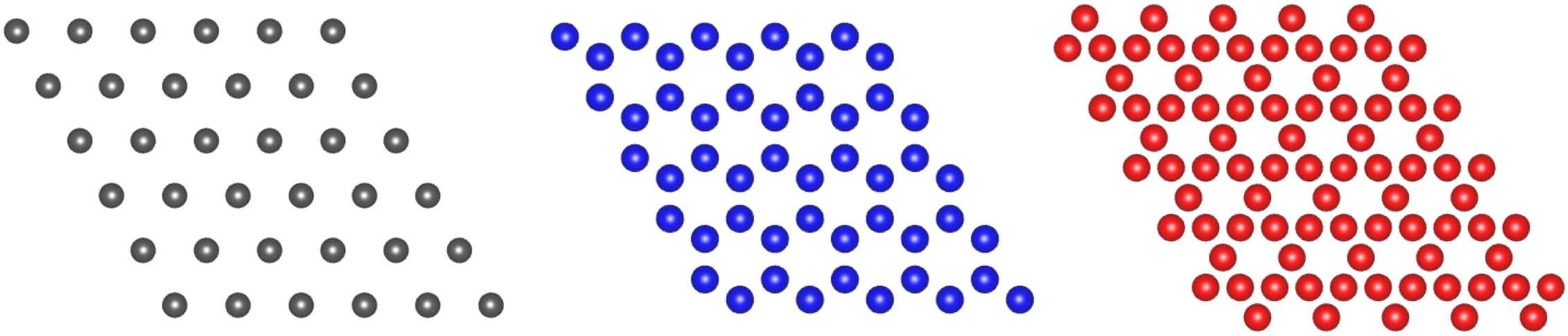
Image: 1605.06824 Ma et al

Link real space orbitals sitting on lattice sites to electronic bands (without a Hamiltonian)?

Band Representation (BR): set of **bands linked to a localized orbital**
(respecting all the crystal symmetries and TRS)

Zak PRB 26 (1982)

Induction of a (P)EBR



1 atom/unit cell
(triangular)

2 atoms/unit cell
(honeycomb)

3 atoms/unit cell
(kagome)

1a

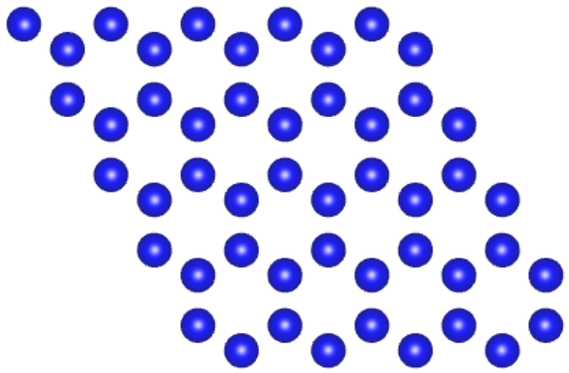
2b

3c

- Within the same SG many ways to arrange atoms
- Each arrangement determines different representations

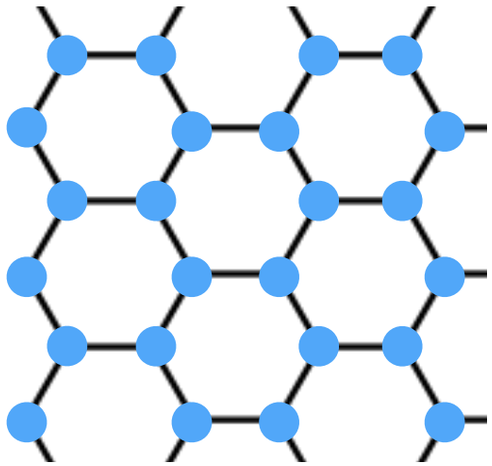
Induction of a (P)EBR

- Within the same lattice, different orbitals

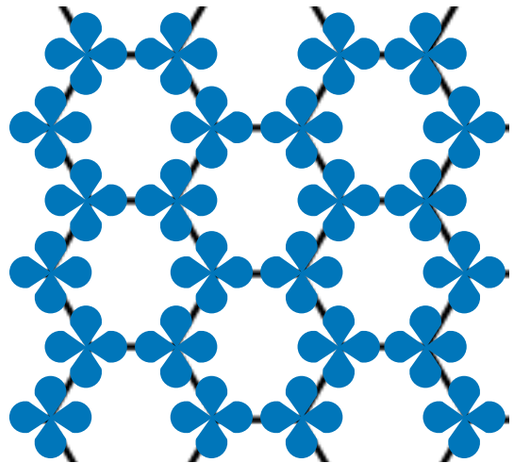


2 atoms/unit cell

s (or p_z) orbitals



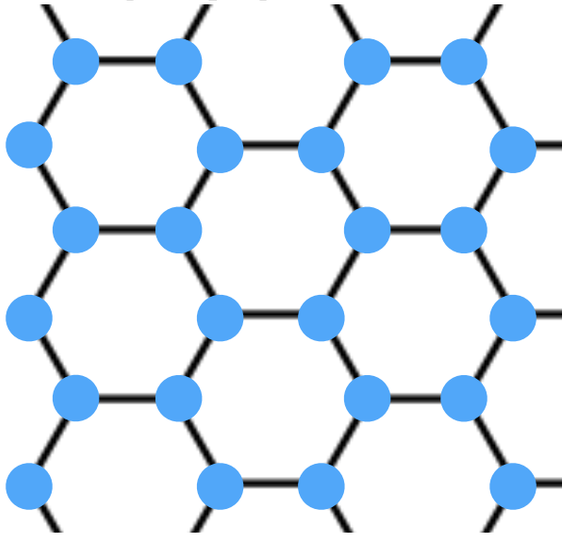
p_x and p_y orbitals



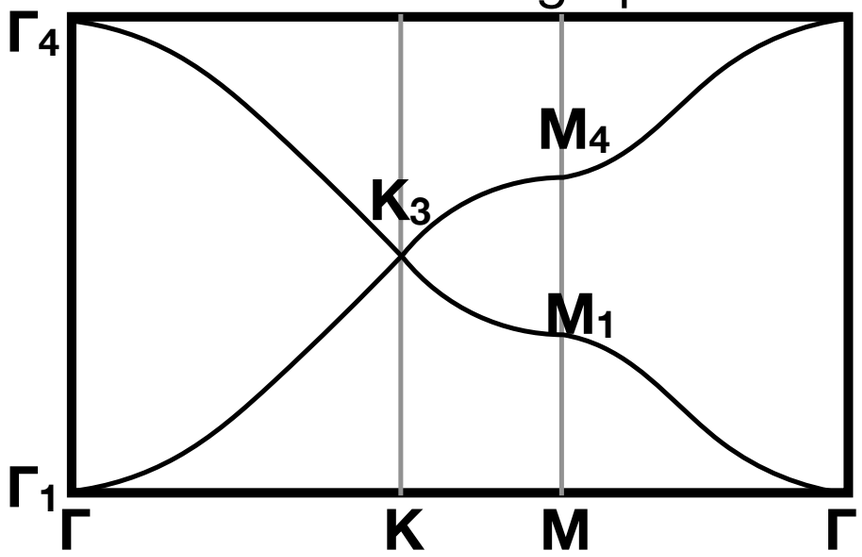
Induction of a (P)EBR

Site-symmetry group, G_q, leaves q invariant

s (or p_z) orbitals



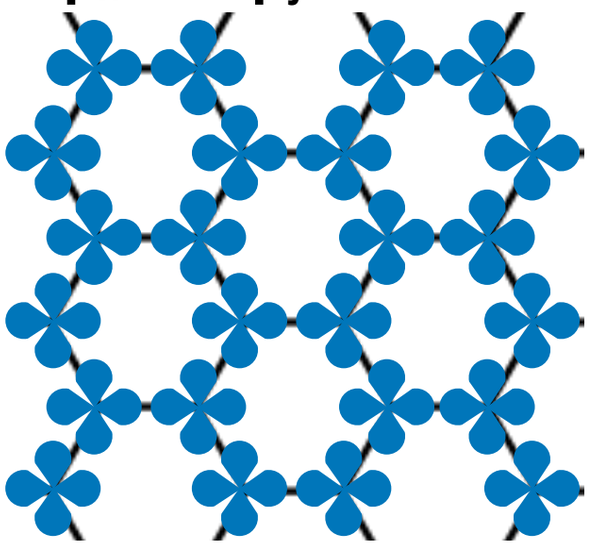
Band structure graphene



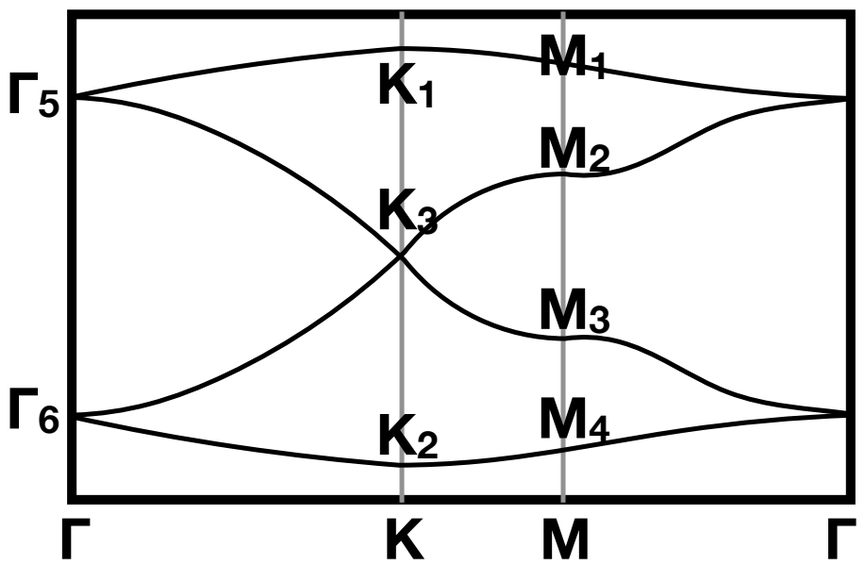
Site-Symmetry group

Real space vs momentum space

p_x and p_y orbitals



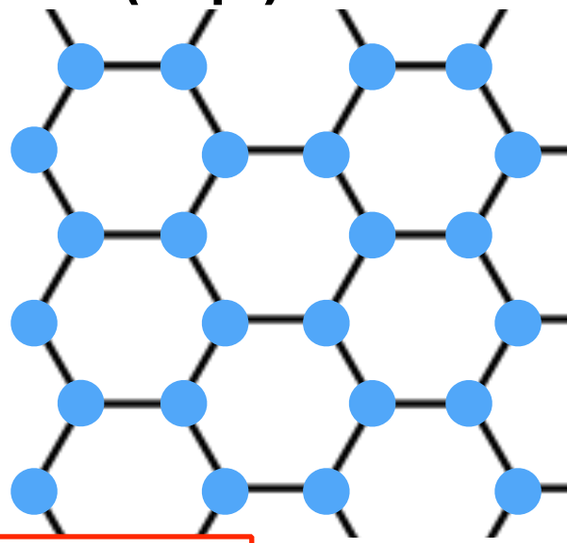
Band structure bismuthene



Induction of a (P)EBR

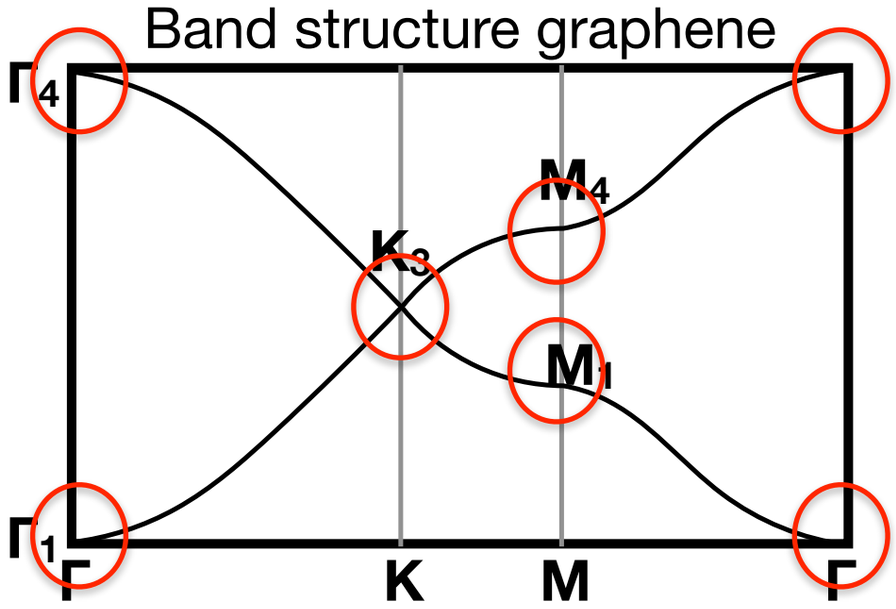
Each arrangement/orbital determines symmetry representations in the Brillouin zone

s (or p_z) orbitals



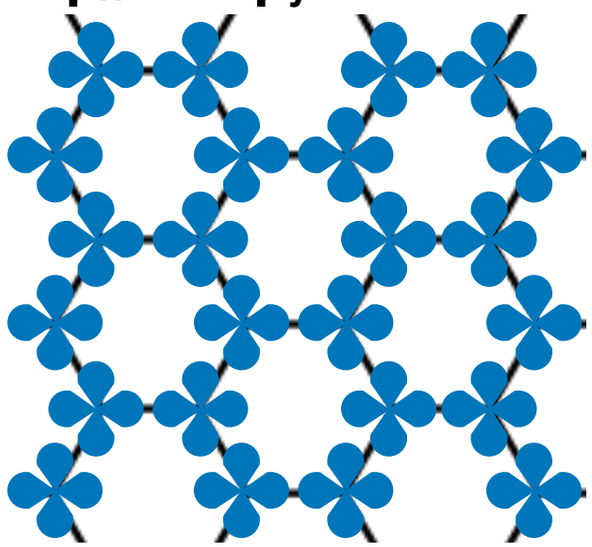
Site-Symmetry group

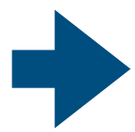
Band structure graphene



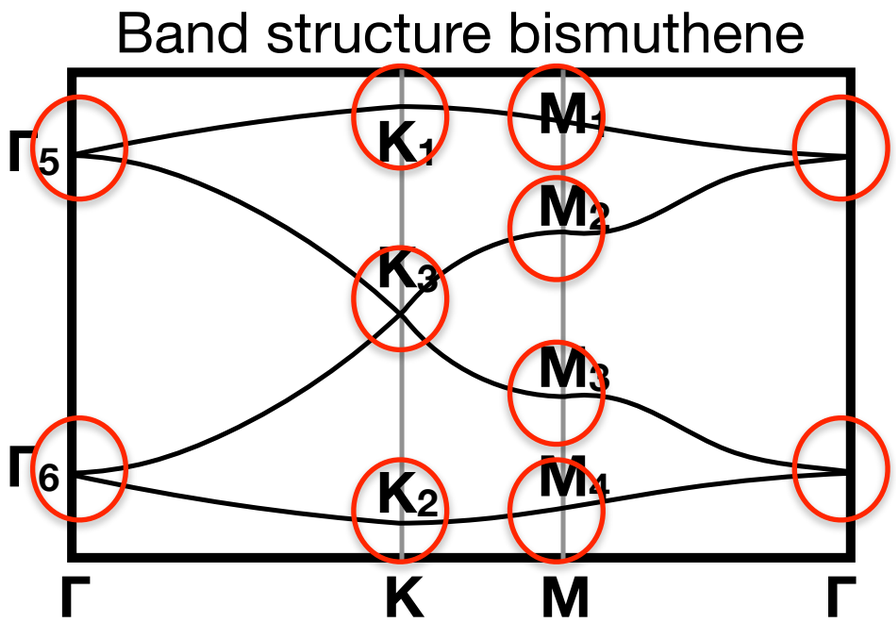
Real space vs momentum space

p_x and p_y orbitals



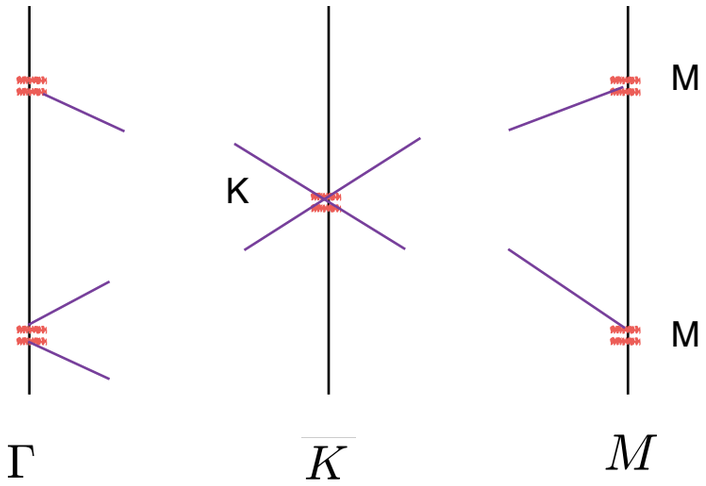


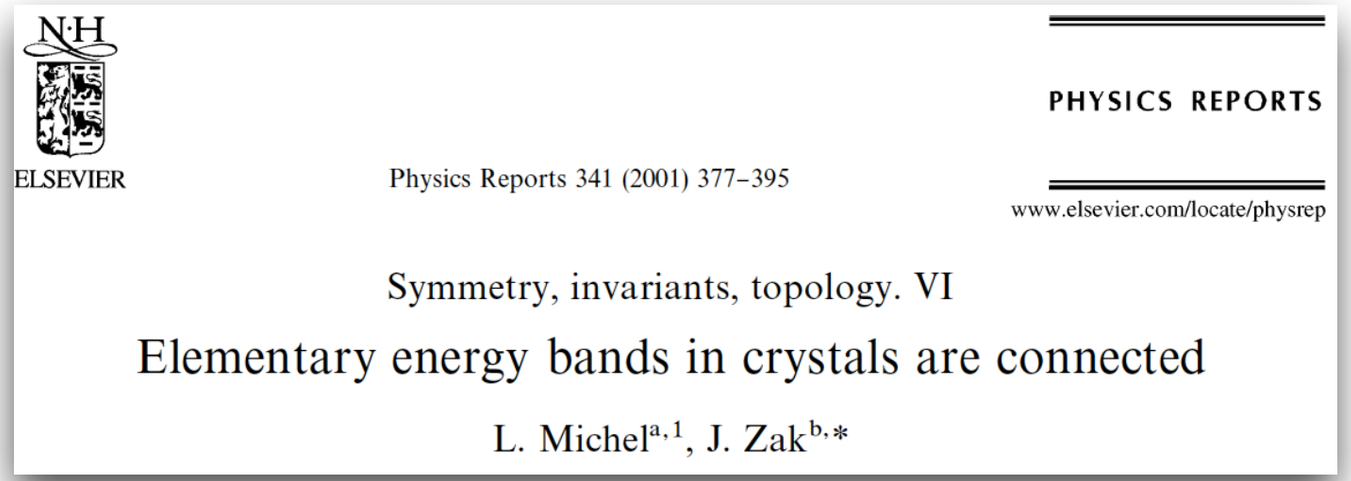
Band structure bismuthene



ATOMIC LIMIT AND WANNIER AS A FUCNTION OF EBRS

- Restricting to the little group at k to find irreps at each k point (subduction) -> **all bands connected**
- EBR is defined by a **maximal Wyckoff position and the irreps in real space**





- **Topology?**

By construction, a **band representation has an atomic limit**,
and all atomic limits yield a band representation*

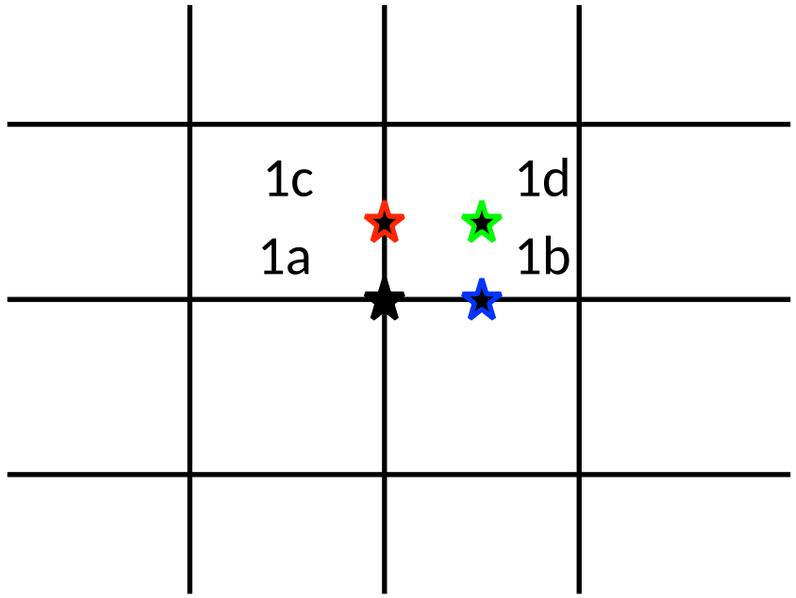
↕

Recall: **Topological bands** **CANNOT Have Maximally Localized** Wannier Function

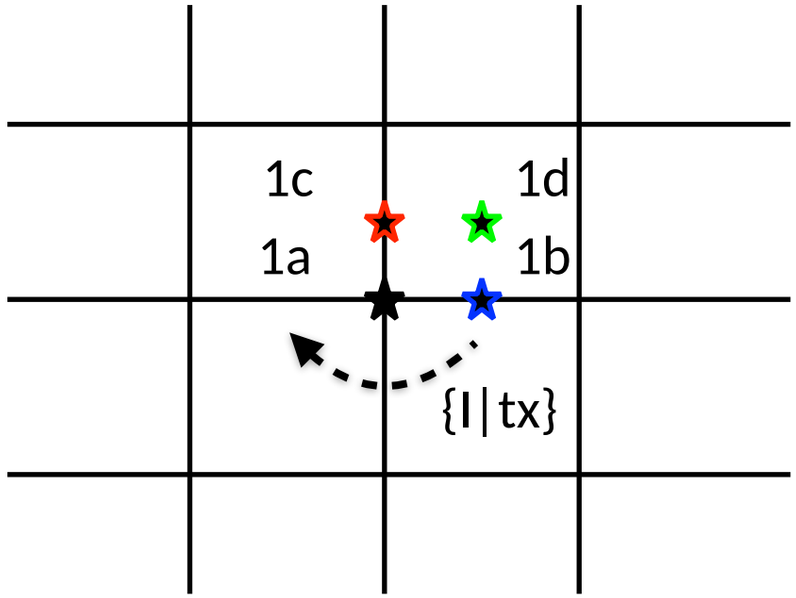
Hence if we know the atomic limits, we know the topological states

Soluyanov and Vanderbilt

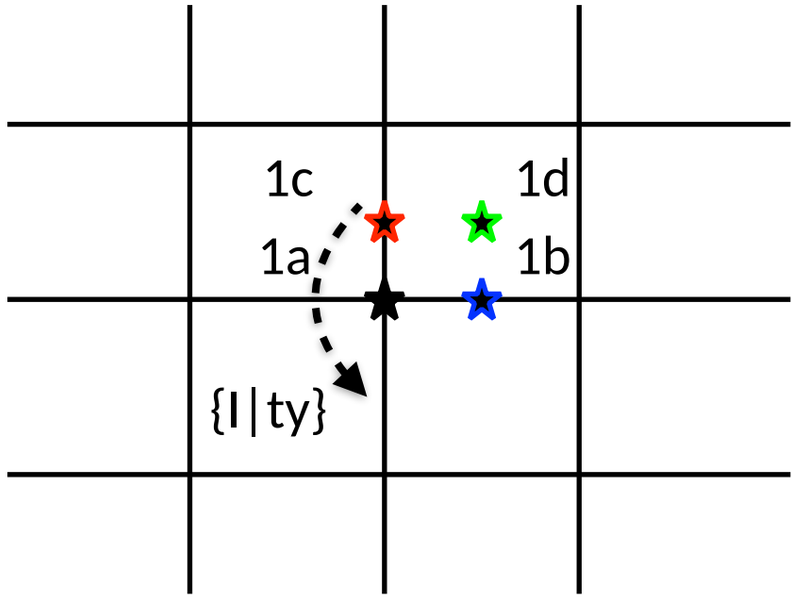
Spinless 2D material, l, s and p orbitals



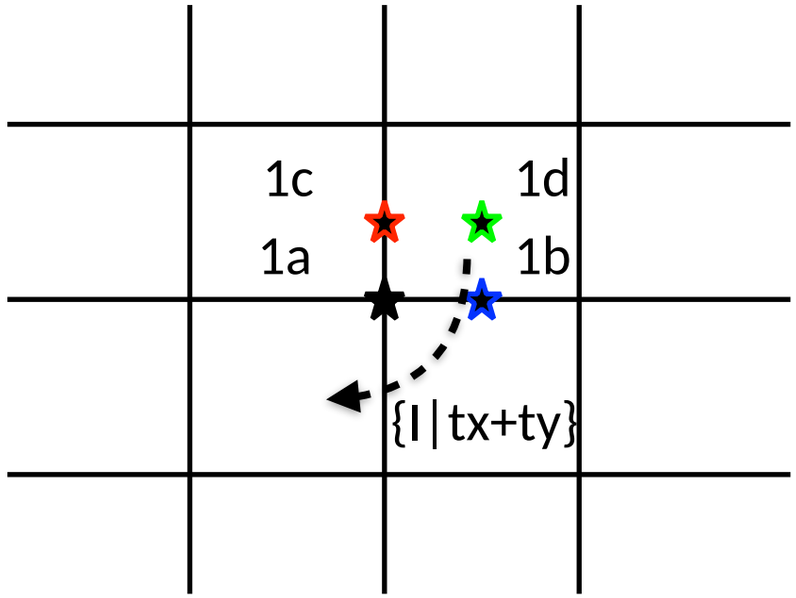
Spinless 2D material, I, s and p orbitals



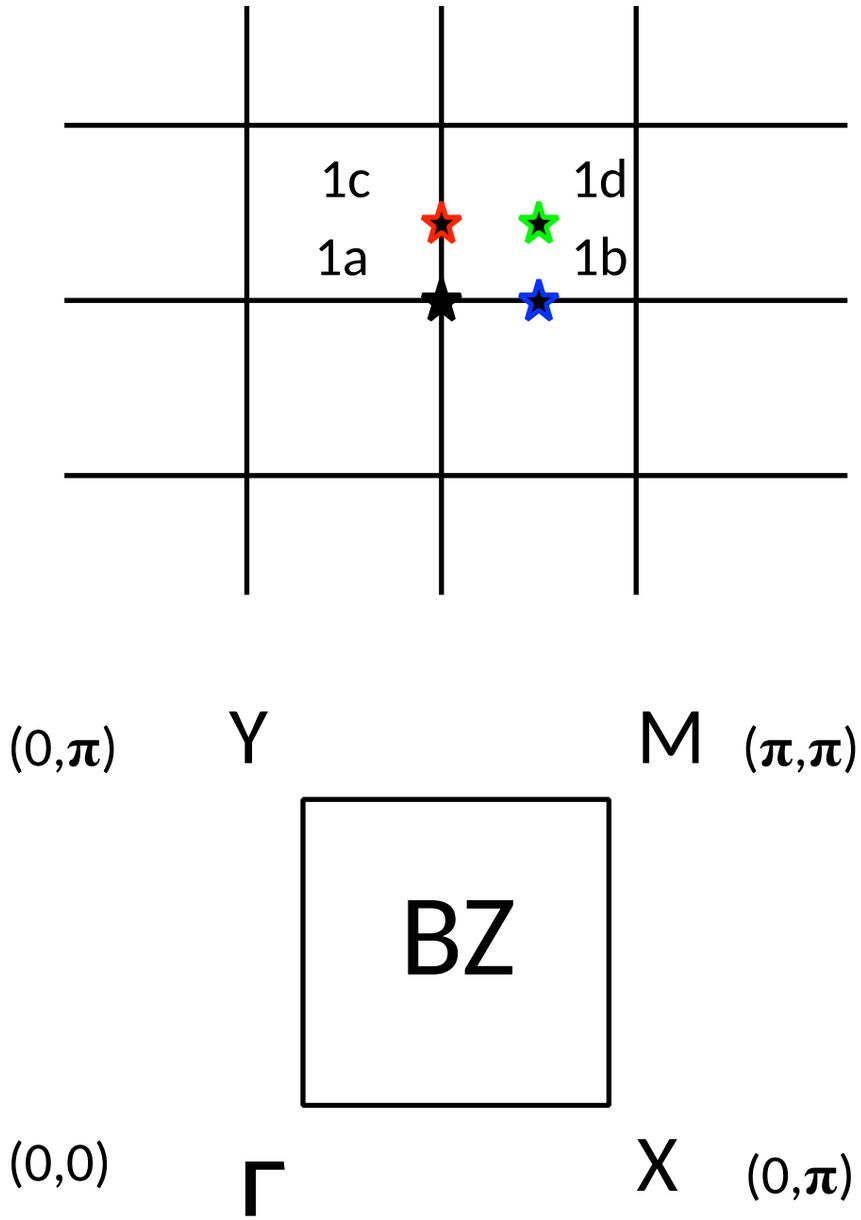
Spinless 2D material, I, s and p orbitals



Spinless 2D material, I, s and p orbitals



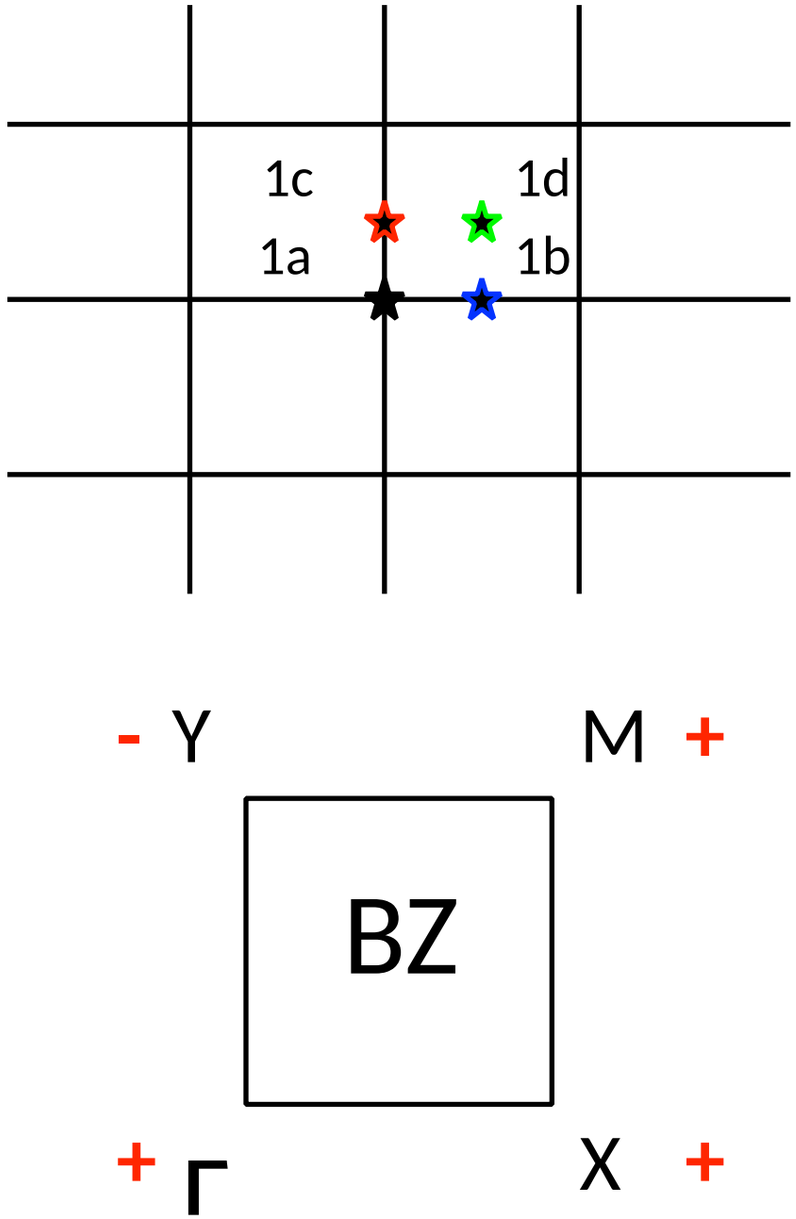
Spinless 2D material, l, **s** and **p** orbitals



	Γ	X	Y	M
s 1a	+	+	+	+
p 1a	-	-	-	-
s 1b	+	-	+	-
p 1b	-	+	-	+
s 1c	+	+	-	-
p 1c	-	-	+	+
s 1d	+	-	+	-
p 1d	-	+	+	-

e^{ik}

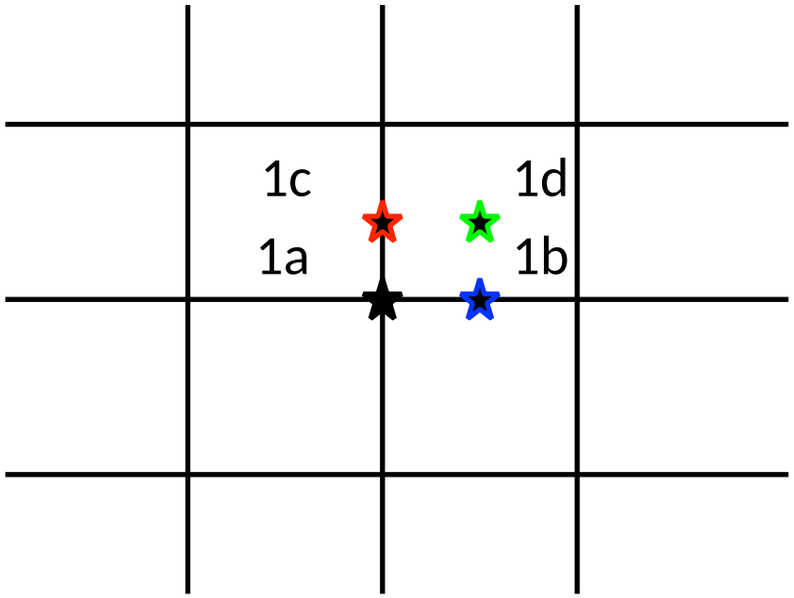
Spinless 2D material, I, s and p orbitals

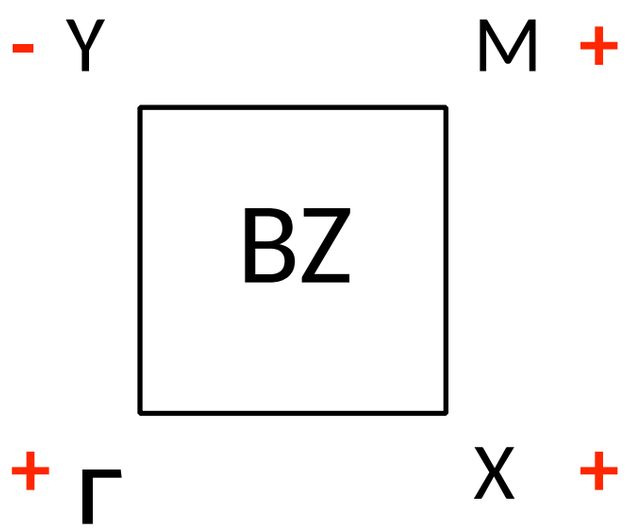


odd # in I eigenvalues

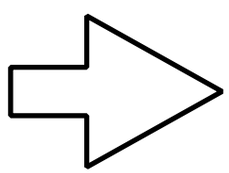
	Γ	X	Y	M
s 1a	+	+	+	+
p 1a	-	-	-	-
s 1b	+	-	+	-
p 1b	-	+	-	+
s 1c	+	+	-	-
p 1c	-	-	+	+
s 1d	+	-	+	-
p 1d	-	+	+	-

Spinless 2D material, I, s and p orbitals





odd # in I eigenvalues



TOPOLOGICAL

	Γ	X	Y	M
s 1a	+	+	+	+
p 1a	-	-	-	-
s 1b	+	-	+	-
p 1b	-	+	-	+
s 1c	+	+	-	-
p 1c	-	-	+	+
s 1d	+	-	+	-
p 1d	-	+	+	-

Full classification of atomic phases

10398 real-space **atomic limits** of non-magnetic materials (groups)

Bilbao Crystallographic Server → BANDREP Help

Band representations of the Double Space Groups

Band Representations

This program calculates the band representations (BR) induced from the irreps of the site-symmetry group of a given Wyckoff position.
Alternatively, it gives the set of elementary BRs of a Double Space Group.
In both cases, it can be chosen to get the BRs with or without time-reversal symmetry.
The program also indicates if the elementary BRs are decomposable or indecomposable. If it is decomposable, the program gives all the possible ways to decompose it.

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A — choose it

1. Get the elementary BRs without time-reversal symmetry — Elementary
2. Get the elementary BRs with time-reversal symmetry — Elementary TR
3. Get the BRs without time-reversal symmetry from a Wyckoff position — Wyckoff
4. Get the BRs with time-reversal symmetry from a Wyckoff position — Wyckoff TR

Bilbao Crystallographic Server
http://www.cryst.ehu.es

For comments, please mail to
administrador.bsc@ehu.eus

http://www.cryst.ehu.es/cryst/bandrep

Nature 547, 298--305 (2017)

SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE	SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE
1	1*a*	1	1	Γ_1	1	1	1	1	*e*	*e*	131	2*d*	2	8	Γ_2^-	1	1	2	1	*e*	*e*
1	1*a*	1	1	$\bar{\Gamma}_2$	1	2	2	2	*e*	*e*	131	2*d*	2	8	Γ_4^+	1	1	2	1	*e*	*e*
2	1*a*	1	2	Γ_1^+	1	1	1	1	*e*	*e*	131	2*d*	2	8	Γ_4^-	1	1	2	1	*e*	*e*
2	1*a*	1	2	Γ_1^-	1	1	1	1	*e*	*e*	131	2*d*	2	8	Γ_3^+	1	1	2	1	*e*	*e*
2	1*a*	1	2	$\bar{\Gamma}_3$	1	2	2	2	*e*	*e*	131	2*d*	2	8	Γ_3^-	1	1	2	1	*e*	*e*
2	1*a*	1	2	$\bar{\Gamma}_2$	1	2	2	2	*e*	*e*	131	2*d*	2	8	$\bar{\Gamma}_5$	2	1	4	1	*e*	*e*
2	1*b*	1	2	Γ_1^+	1	1	1	1	*e*	*e*	131	2*d*	2	8	$\bar{\Gamma}_6$	2	1	4	1	*e*	*e*
2	1*b*	1	2	Γ_1^-	1	1	1	1	*e*	*e*	131	2*e*	2	14	Γ_1	1	1	2	1	*e*	*e*
2	1*b*	1	2	$\bar{\Gamma}_3$	1	2	2	2	*e*	*e*	131	2*e*	2	14	Γ_4	1	1	2	1	*e*	*e*

12b(2)	8a(3)	8a(3)	12b(2)
B↑G(6)	$^1\bar{E}^2\bar{E}$↑G(8)	$\bar{E}\bar{E}$↑G(8)	$^1\bar{E}^2\bar{E}$↑G(12)
Indecomposable	Indecomposable	Decomposable	Decomposable
2 Γ_4(3)	2 $\bar{\Gamma}_5$(2) ⊕ $\bar{\Gamma}_6\bar{\Gamma}_7$(4)	2 $\bar{\Gamma}_6\bar{\Gamma}_7$(4)	2 $\bar{\Gamma}_5$(2) ⊕ 2 $\bar{\Gamma}_6\bar{\Gamma}_7$(4)
H_1(1) ⊕ H_2H_3(2) ⊕ H_4(3)	2 $\bar{H}_5$(2) ⊕ $\bar{H}_6\bar{H}_7$(4)	2 $\bar{H}_6\bar{H}_7$(4)	2 $\bar{H}_5$(2) ⊕ 2 $\bar{H}_6\bar{H}_7$(4)
P_1(2) ⊕ P_2(2) ⊕ P_3(2)	$\bar{P}_5$(1) ⊕ $\bar{P}_6$(1) ⊕ 2 $\bar{P}_7$(3)	2 $\bar{P}_4$(1) ⊕ 2 $\bar{P}_7$(3)	$\bar{P}_4$(1) ⊕ $\bar{P}_5$(1) ⊕ $\bar{P}_6$(1) ⊕ 3 $\bar{P}_7$(3)
PA_1(2) ⊕ PA_2(2) ⊕ PA_3(2)	$\overline{PA}_5$(1) ⊕ $\overline{PA}_6$(1) ⊕ 2 $\overline{PA}_7$(3)	2 $\overline{PA}_4$(1) ⊕ 2 $\overline{PA}_7$(3)	$\overline{PA}_4$(1) ⊕ $\overline{PA}_5$(1) ⊕ $\overline{PA}_6$(1) ⊕ 3 $\overline{PA}_7$(3)
3 N_1(1) ⊕ 3 N_2(1)	4 $\bar{N}_3\bar{N}_4$(2)	4 $\bar{N}_3\bar{N}_4$(2)	6 $\bar{N}_3\bar{N}_4$(2)

Materials search

Topological “insulating” classes { EBR1, EBR2

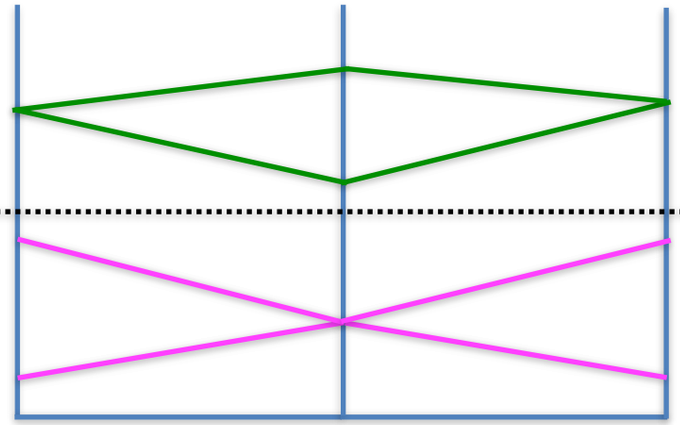
b=$\sum_m a_m$ EBR=a1*ebr1+a2*ebr2….

if a_m positive integer : trivial

else : topological

LCEBR

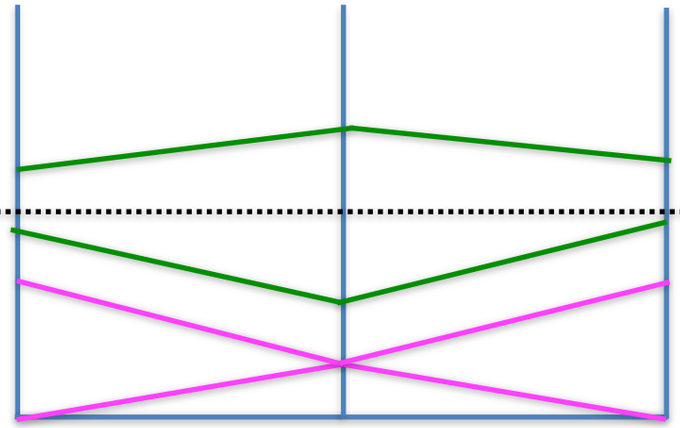
Linear Combination EBR



b=EBR1

SEBR

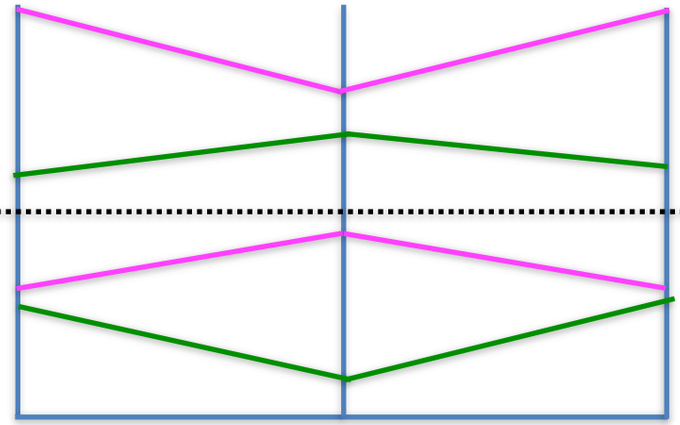
Split EBR



b=EBR1+1/2*EBR2

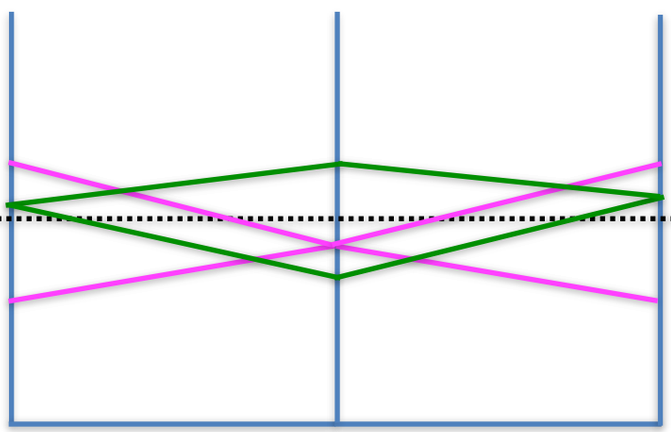
NLC

Non Linear Combination

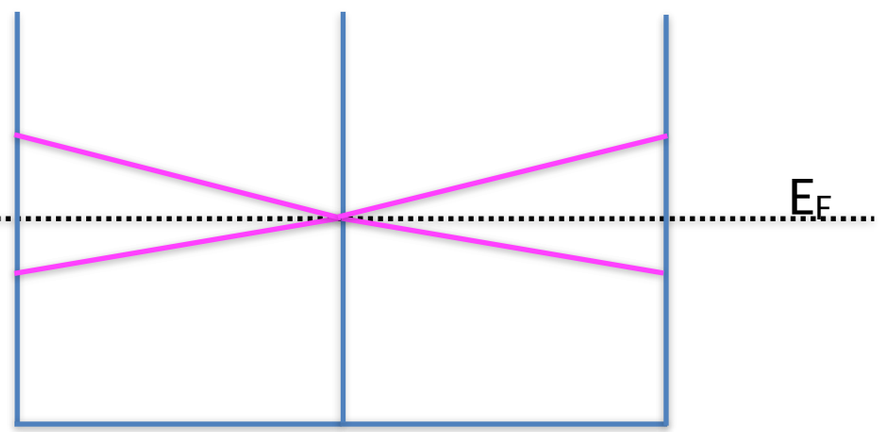


b = 1/2*EBR1+1/2*EBR2

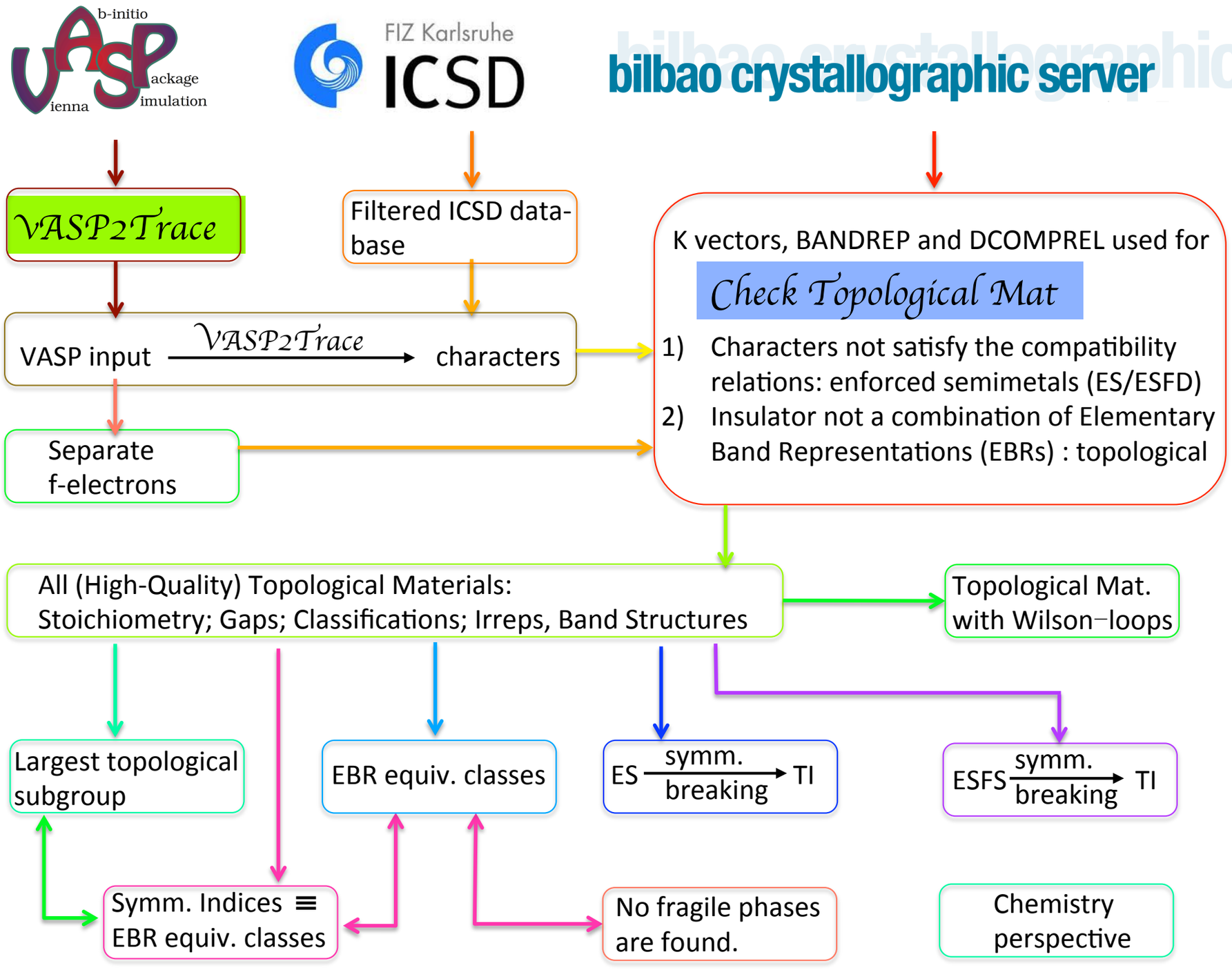
ES: Enforced semimetals



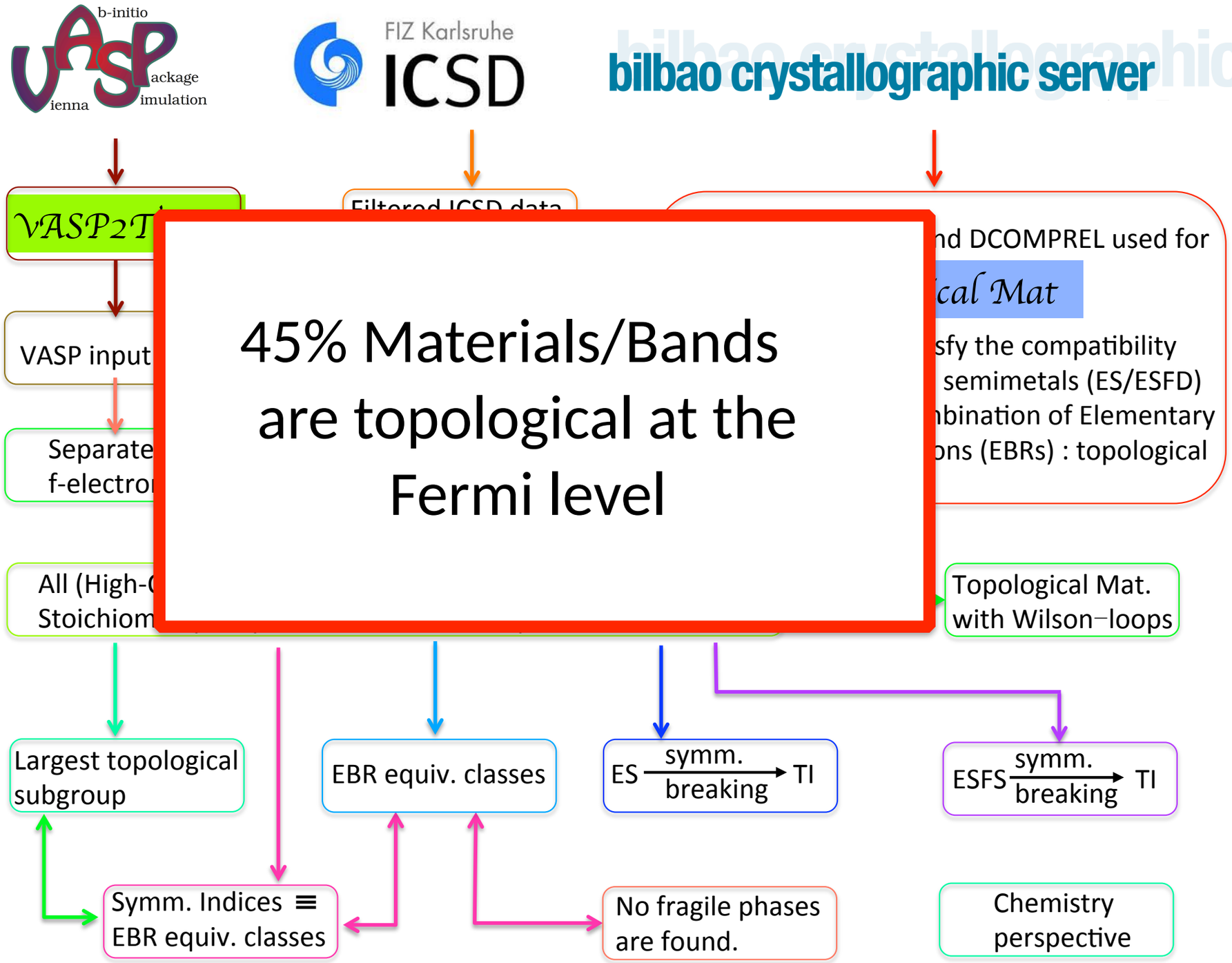
ESFD: ES Fermi Degeneracy



Materials search

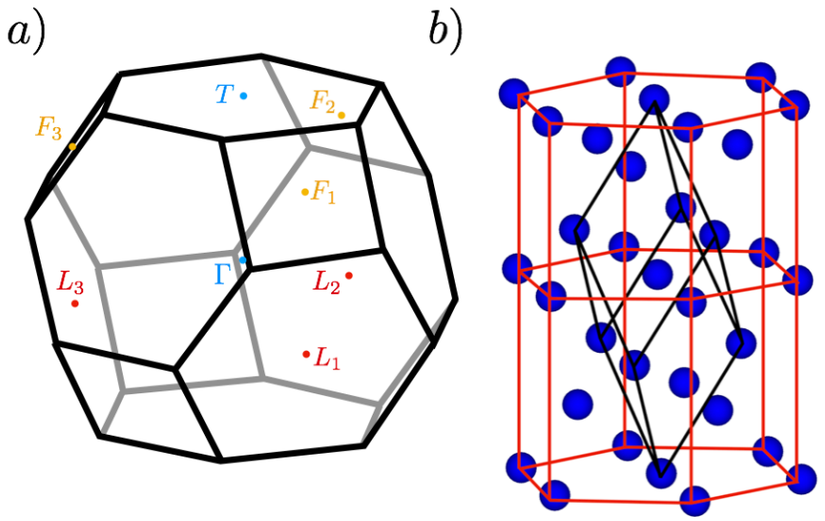


Materials search



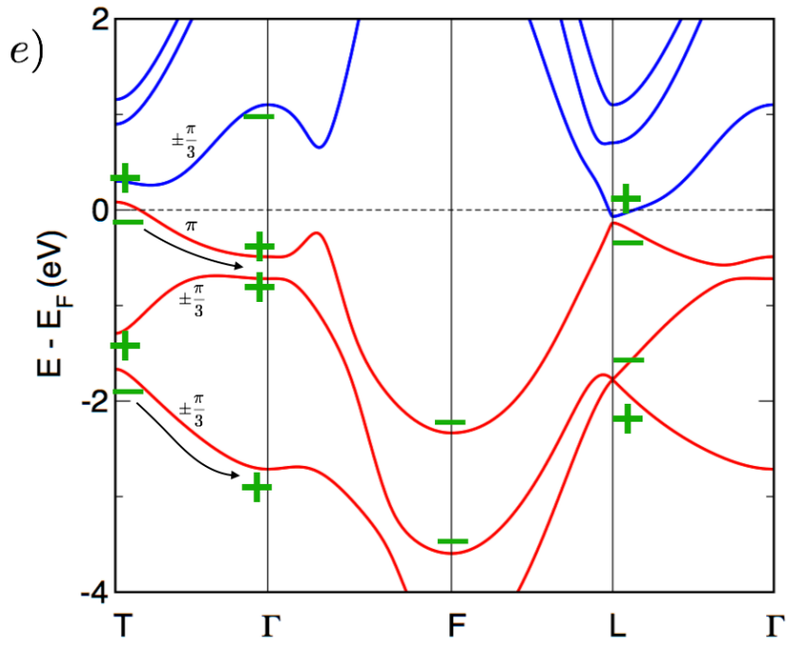
Nature 566, 480-485 (2019), Song arXiv:1905.03262

High Order TI in terms of EBRs: The case of Bi

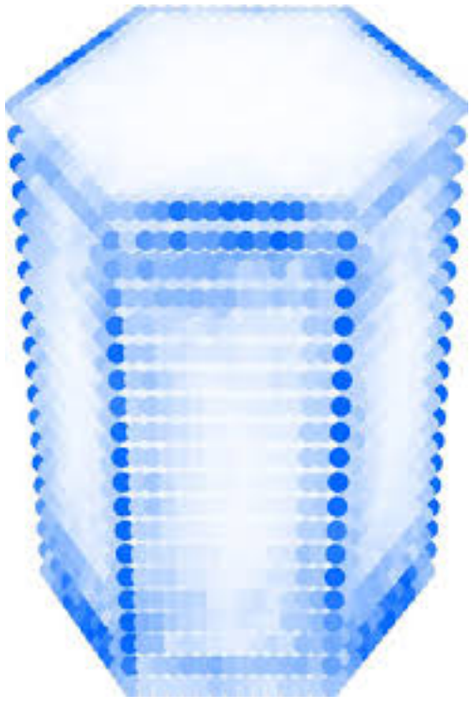


pEBRs of SG 166 with TRS

	F	Γ	L	T
$3a$				
$\bar{\Gamma}^{3a}_{4+5} \uparrow G$	$\bar{F}_3\bar{F}_4$	$\bar{\Gamma}_4\bar{\Gamma}_5$	$\bar{L}_3\bar{L}_4$	$\bar{T}_4\bar{T}_5$
$\bar{\Gamma}^{3a}_{6+7} \uparrow G$	F_5F_6	$\Gamma_6\Gamma_7$	$\bar{L}_5\bar{L}_6$	$\bar{T}_6\bar{T}_7$
$\bar{\Gamma}^{3a}_{8} \uparrow G$	$\bar{F}_3\bar{F}_4$	$\bar{\Gamma}_8$	$\bar{L}_3\bar{L}_4$	$\bar{T}_8$
$\bar{\Gamma}^{3a}_{9} \uparrow G$	F_5F_6	Γ_9	$\bar{L}_5\bar{L}_6$	$\bar{T}_9$
$3b$				
$\bar{\Gamma}^{3b}_{4+5} \uparrow G$	$\bar{F}_3\bar{F}_4$	$\bar{\Gamma}_4\bar{\Gamma}_5$	$\bar{L}_5\bar{L}_6$	$\bar{T}_6\bar{T}_7$
$\bar{\Gamma}^{3b}_{6+7} \uparrow G$	F_5F_6	$\Gamma_6\Gamma_7$	$\bar{L}_3\bar{L}_4$	$\bar{T}_4\bar{T}_5$
$\bar{\Gamma}^{3b}_{8} \uparrow G$	$\bar{F}_3\bar{F}_4$	$\bar{\Gamma}_8$	$\bar{L}_5\bar{L}_6$	$\bar{T}_9$
$\bar{\Gamma}^{3b}_{9} \uparrow G$	F_5F_6	Γ_9	$\bar{L}_3\bar{L}_4$	$\bar{T}_8$



Bi, $\bar{R}$3m SG (6c Wyckoff position)



computed pEBRs of Bi

	3 doubly-degenerate valence bands
F	$\bar{F}_3\bar{F}_4;\ F_5F_6;\ \bar{F}_5\bar{F}_6$
Γ	$\bar{\Gamma}_8;\ \bar{\Gamma}_8;\ \bar{\Gamma}_4\bar{\Gamma}_5$
L	$\bar{L}_3\bar{L}_4;\ L_5L_6;\ L_5L_6$
T	$\bar{T}_9;\ \bar{T}_8;\ \bar{T}_6\bar{T}_7$

Nat. Phys. (2018)

SUPERTOPOLOGY

Question: How many bands do we need to “change” to get to an atomic limit
Answer: All??! Then material is super topological

All bands below Fermi for Bi are topological

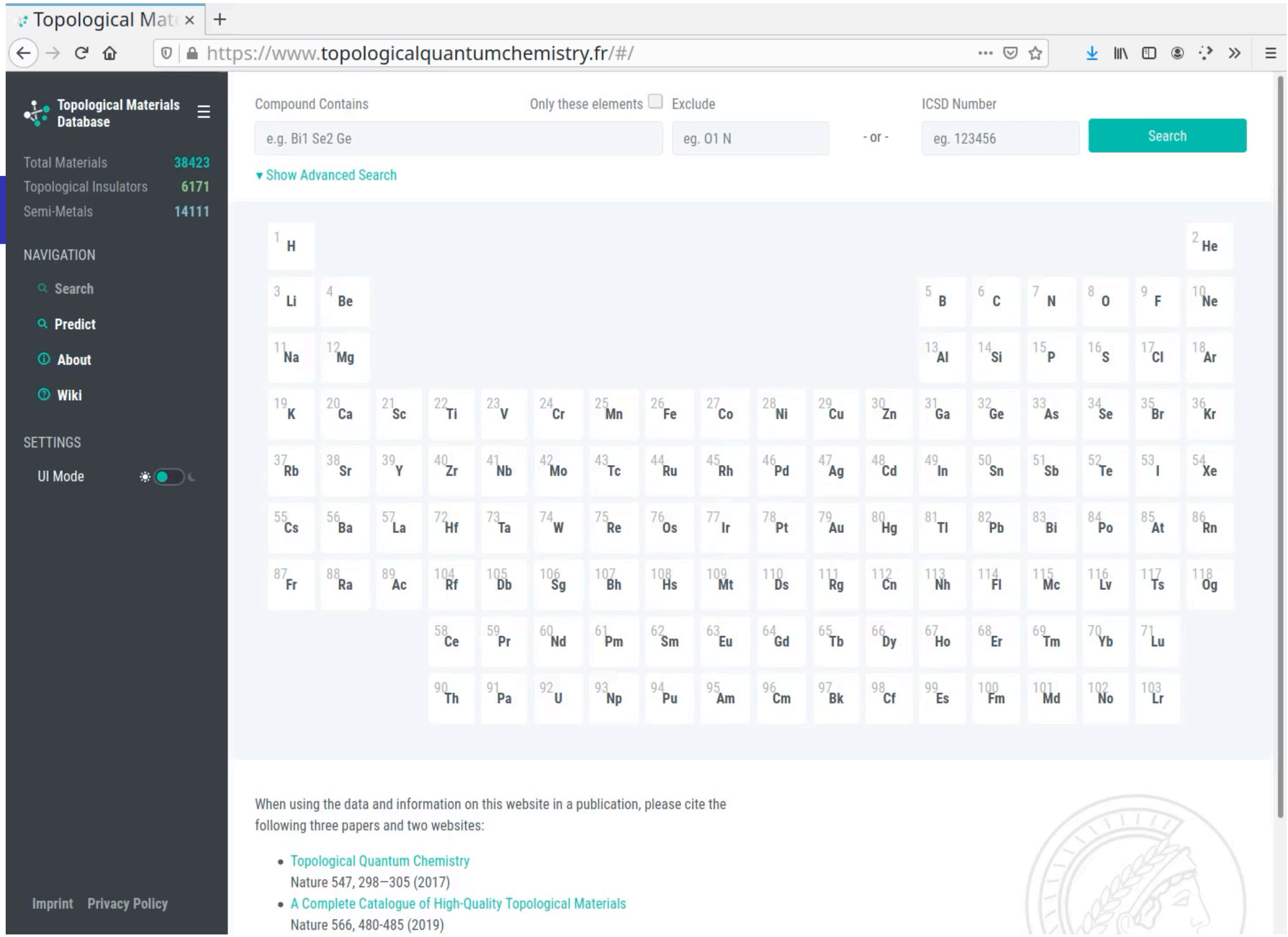
Nbr Bands	Subclass	Γ	T	F	L
2	SEBR	8 (1)	9 (1)	5+6 (1)	3+4 (1)
2	SEBR	9 (1)	8 (1)	3+4 (1)	5+6 (1)
2	SEBR	8 (1)	9 (1)	3+4 (1)	3+4 (1)
2	SEBR	8 (1)	8 (1)	5+6 (1)	5+6 (1)
2	SEBR	4+5 (1)	6+7 (1)	5+6 (1)	5+6 (1)
2	SEBR	9 (1)	8 (1)	3+4 (1)	3+4 (1)
2	SEBR	9 (1)	9 (1)	3+4 (1)	3+4 (1)
2	SEBR	6+7 (1)	4+5 (1)	3+4 (1)	5+6 (1)
2	SEBR	9 (1)	9 (1)	5+6 (1)	3+4 (1)

830 compounds show supertopology

to appear soon

Sneak Preview: New Website, All Materials With < 70 Atoms/Unit cell

- Improved U.I..
- *More than 38k unique materials* (71k unique ICSDs).
- With and without SOC.
- Dynamical plots.
- Fragile phases.
- Wiki and more.



Topological Materials Database

https://www.topologicalquantumchemistry.com

Check Topology

www.cryst.ehu.es/cryst/checktopologicalmat

Check Topological Mat

Check Topological Mat.

Given a file that contain the eigenvalues at each maximal k-vec of a space group, the program gives the set of irreducible representations at each maximal k-vec (time-reversal is assumed). Then, using the compatibility relations and the set of Elementary Band Representations (EBRs), it checks whether the set of bands can be put as linear combinations of EBRs. This (self-explanatory) file shows the format of the file to be uploaded in the menu on the right:

File_Description

You can download examples of input files here:

Example_Ag1Ge1Li2 Example_Ag1O2Sc1
Example_B2Ca3Ni7 Example_Ba3Co10O17
Example_Ba3Ca1O9Ru2

You can generate the "trace.txt" file in your own computer using VASP and this program (fortran).

vasp2trace

Read the "README.pdf" file for help on the use of vasp2trace.
If you are using "Check Topological Mat." and/or "vasp2trace" programs in the preparation of an article, please cite this reference:

M.G. Vergniory, L. Elcoro, C. Felser, B.A. Bernevig, Z. Wang (2018) arXiv:1807.10271

Upload your traces.txt file

Browse... No file selected.

Show

```
Number of electrons=10
Number of maximal k-vectors=4
Symbols of the k-vectors, number of bands up to fermi level and set of irreps.
     -GM      -X         -L      -W
      10      10         10      10
 -GM6(2) -X6(2)     -L9(2) -W6(2)
 -GM6(2) -X6(2)     -L8(2) -W7(2)
 -GM8(2) -X8(2)     -L8(2) -W7(2)
-GM11(4) -X8(2) -L4-L5(2) -W6(2)
         -X9(2)     -L9(2) -W7(2)
```

- The material is a topological insulator.
- List of topological indices:

  z2w,1=0

  z2w,2=0

  z2w,3=0

  z4=0

  z2=0

  z8=4

- The material belongs to the strong topological class: 1
- Clicking on See the irreps you can see the details about the number of bands and the ide
- The set of bands can be put as linear combination of Elementary Band Representations (I to get some possible linear combinations of EBRs and partial EBRs.
- Click on Subgroups to check the topological character of the structure in each of its (trans

1. A number of bands that is **not a sum of EBRs is topological**
2. A number of bands that does **not satisfy the compatibility relations** cannot be separated from other bands and describes a **semimetal**

Nature 566, 480-485 (2019)

Magnetic Materials

- Magnetic materials can also be topological
  - Case-by-case evaluation
  - QAH, AFM TI, Magnetic Weyl, “Axion” Insulators (AXIs)

Haldane, *PRL* (1988)
Mong, Essin, Moore, *PRB* (2010)
Hughes, Prodan, Bernevig, *PRB* (2010)
Wan, Turner, Vishwanath, Savrasov, *PRB* (2011)

- Significant Computational complications
  - Is mean-field-theory valid? (bands?)
  - Is magnetic order measured (magnetic order prediction is hard)?
  - Is magnetism commensurate?
  - **If all the above yes, still very hard!**
  - Must compute electronic structrure
  - Must have full theory of magnetic topology: not even full representations are derived

Is this a topological magnet??

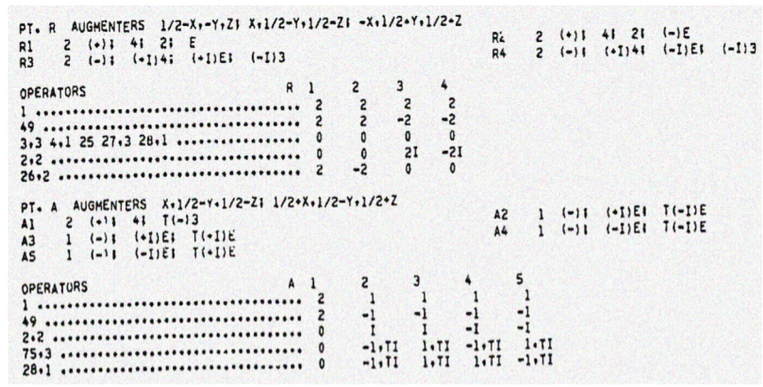
Magnetic Symmetry and Group Theory

Assume: <u>bands exist, magnetic structure is known, commensurate</u>

- Many, many magnetic symmetry groups (1421 MSGs vs. 230 SGs)
- Magnetic order ≠ MSG

- Full magnetic coreps/irreps are inaccessible
- Magnetic compatibility relations aren't known
- Magnetic trivial bands (MEBRs) aren't known
- Magnetic eigenvalue indicators (topological indices) aren't known

Some coreps in Fortran tables:
Miller and Love (1967)



PT. R AUGMENTERS 1/2-X,-Y,Z; X,1/2-Y,1/2-Z; -X,1/2+Y,1/2+Z

R1 2 (+)E 4I 2I E
R3 2 (-)E (+I)4; (+I)E; (-I)3

R4 2 (+)E 4I 2I (-)E
R4 2 (-)E (+I)4I (-I)E; (-I)3

OPERATORS R	1	2	3	4
1	2	2	2	2
49	2	2	-2	-2
3,3 4,1 25 27,3 28,1	0	0	0	0
2,2	0	0	2I	-2I
26,2	2	-2	0	0

PT. A AUGMENTERS X,1/2-Y,1/2-Z; 1/2+X,1/2-Y,1/2+Z

A1 2 (+)E 4I T(-)3
A3 1 (-)E (+I)E; T(+I)E
A5 1 (-)E (-I)E; T(+I)E

A2 1 (-)E (+I)E; T(-I)E
A4 1 (-)E (-I)E; T(-I)E

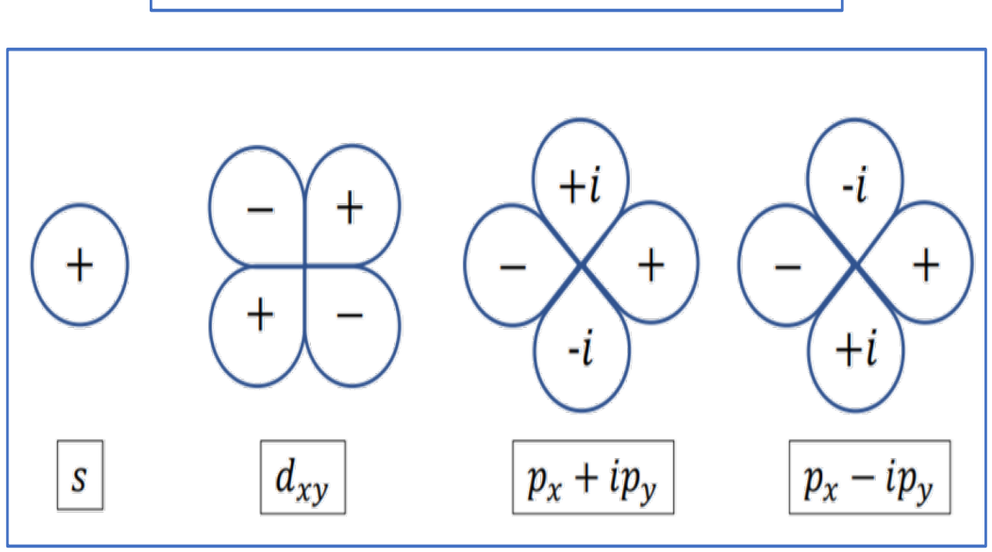
OPERATORS A	1	2	3	4	5
1	2	1	1	1	1
49	2	-1	-1	-1	-1
2,2	0	I	I	-I	-I
75,3	0	-1,TI	1,TI	-1,TI	1,TI
28,1	0	-1,TI	1,TI	1,TI	-1,TI

MSG indicator groups (not indices) (*e.g.* $\mathbb{Z}_2\times\mathbb{Z}_2$): Watanabe, Po, Vishwanath, *Sci. Adv.* (2018)

Magnetic Topological Quantum Chemistry

- Complete theory of mean-field magnetic topology
- **MTQC** subsumes **TQC** (230 SGs + 1421 MSGs = 1651 SSGs)
  - Calculate **all** magnetic coreps and all **33021** (M)EBRs

Magnetic atomic orbitals



Magnetic Coreps and MEBRs Soon Freely Accessible on Bilbao Crystallographic Server

Wyckoff pos.		1a(2',1)	1a(2',1)	1b(2',1)	1b(2',1)	1c(2',1)	1c(2',1)	1d(2',1)	1d(2',1)
Band-rep.		A↑G(1)	$\bar{A}$↑G(1)	A↑G(1)	$\bar{A}$↑G(1)	A↑G(1)	$\bar{A}$↑G(1)	A↑G(1)	$\bar{A}$↑G(1)
Decomposable \Indecomposable		Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable
Γ:(0,0,0)	Γ':(0,0,0)	$\Gamma_1(1)$	$\bar{\Gamma}_2(1)$	$\Gamma_1(1)$	$\bar{\Gamma}_2(1)$	$\Gamma_1(1)$	$\bar{\Gamma}_2(1)$	$\Gamma_1(1)$	$\bar{\Gamma}_2(1)$
A:(1/2,0,1/2)	U:(1/2,0,1/2)	$(A)U_1(1)$	$(A)\bar{U}_2(1)$	$(A)U_1(1)$	$(A)\bar{U}_2(1)$	$(A)U_1(1)$	$(A)\bar{U}_2(1)$	$(A)U_1(1)$	$(A)\bar{U}_2(1)$
B:(0,0,1/2)	Z:(0,0,1/2)	$(B)Z_1(1)$	$(B)\bar{Z}_2(1)$	$(B)Z_1(1)$	$(B)\bar{Z}_2(1)$	$(B)Z_1(1)$	$(B)\bar{Z}_2(1)$	$(B)Z_1(1)$	$(B)\bar{Z}_2(1)$
C:(1/2,1/2,0)	V:(1/2,1/2,0)	$(C)V_1(1)$	$(C)\bar{V}_2(1)$	$(C)V_1(1)$	$(C)\bar{V}_2(1)$	$(C)V_1(1)$	$(C)\bar{V}_2(1)$	$(C)V_1(1)$	$(C)\bar{V}_2(1)$
D:(0,1/2,1/2)	T:(0,1/2,1/2)	$(D)T_1(1)$	$(D)\bar{T}_2(1)$	$(D)T_1(1)$	$(D)\bar{T}_2(1)$	$(D)T_1(1)$	$(D)\bar{T}_2(1)$	$(D)T_1(1)$	$(D)\bar{T}_2(1)$
E:(1/2,1/2,1/2)	R:(1/2,1/2,1/2)	$(E)R_1(1)$	$(E)\bar{R}_2(1)$	$(E)R_1(1)$	$(E)\bar{R}_2(1)$	$(E)R_1(1)$	$(E)\bar{R}_2(1)$	$(E)R_1(1)$	$(E)\bar{R}_2(1)$
Y:(1/2,0,0)	X:(1/2,0,0)	$(Y)X_1(1)$	$(Y)\bar{X}_2(1)$	$(Y)X_1(1)$	$(Y)\bar{X}_2(1)$	$(Y)X_1(1)$	$(Y)\bar{X}_2(1)$	$(Y)X_1(1)$	$(Y)\bar{X}_2(1)$
Z:(0,1/2,0)	Y:(0,1/2,0)	$(Z)Y_1(1)$	$(Z)\bar{Y}_2(1)$	$(Z)Y_1(1)$	$(Z)\bar{Y}_2(1)$	$(Z)Y_1(1)$	$(Z)\bar{Y}_2(1)$	$(Z)Y_1(1)$	$(Z)\bar{Y}_2(1)$

- Complete strong and fragile eigenvalue indicators
- **Physical meaning (new TIs) of all electronic indicators!**

- Y. Xu, L. Elcoro, Z. Song, B. J. Wieder, M. G. Vergniory, N. Regnault, Y. Chen, C. Felser, B. A. Bernevig, *arXiv:2003.00012* (2020)
- L. Elcoro*, B. J. Wieder*, Z. Song*, Y. Xu, N. Regnault, B. Bradlyn, B. A. Bernevig, *To Appear*

Magnetic Material Database With Known Structures From Neutron Scattering

bilbao crystallographic server

Structure Databases	
B-IncStrDB	The Bilbao Incommensurate Crystal Structure Database
MAGNDATA	A collection of magnetic structures with transportable cif-type files

MAGNDATA
707 magnetic materials with portable cif-type files

- 95 alloys
- 549 magnetic material candidates with 261 MSGs for ab initio calculations
- 63 materials with Incommensurate structure

- **Crystal and Magnetic structures from experiments.**
- **(Para)Magnetic symmetries**
- **Portable mcif files.**

https://www.cryst.ehu.es

until Jan. 2020

Crystal & Magnetic structures from mcif files

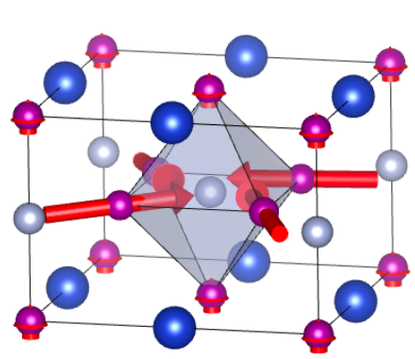
Example: BCSID-2.5

```
_chemical_formula_sum                    'Mn3 Cu N'
_parent_space_group.name_H-M_alt  'P  m  -3m'
_parent_space_group.IT_number                    221
_parent_space_group.child_transform_Pp_abc  'a-b,a+b,c;1/2,1/2,0'
_space_group_magn.transform_BNS_Pp_abc  'b,-a,c;1/4,-1/4,0'
```

Cell Transformations:
from parent unit-cell to mag unit-cell (working setting);
from working setting to standard setting (BNS MSG)

```
_space_group_magn.number_BNS  85.59
_space_group_magn.name_BNS  "P  4/n"
_space_group_magn.point_group_name  "4/m"
_space_group_magn.point_group_number  "11.1.35"
```

→ MSG & MPG



```
_cell_length_a          5.52390
_cell_length_b          5.52390
_cell_length_c          3.90600
_cell_angle_alpha        90.00
_cell_angle_beta         90.00
_cell_angle_gamma        90.00
```

→ Lattice parameters of mag unitcell

```
_space_group_symop_magn_operation.xyz
1 x,y,z,+1
2 -y,x,z,+1
3 y,-x,z,+1
4 -x,-y,z,+1
5 -x+1/2,-y+1/2,-z,+1
6 y+1/2,-x+1/2,-z,+1
7 -y+1/2,x+1/2,-z,+1
8 x+1/2,y+1/2,-z,+1
```

Magn symm. oprs.

+1 : unitary
-1: anti-unitary

```
_atom_site_
Cu1     Cu 0.00000 0.50000 0.00000 1
Mn1_1 Mn 0.75000 0.75000 0.50000 1
Mn1_2 Mn 0.00000 0.00000 0.00000 1
N1      N 0.00000 0.00000 0.50000 1
```

Wyck. pos.
in unit of mag lattice vec.

```
_atom_site_moment
Mn1_1 -2.55 -1.27 0.2 mx,my,mz
Mn1_2 0.0 0.0 0.65 0,0,mz
```

Magn. moments
along mag lattice vec.

Calculational methods: New Package 1 Addition to VASP

Ab-initio calculations are performed with ***VASP*** Package.

- **GGA-PBE** functional method; Spin-orbital coupling (SOC);
- LDA+U; U=0,1,2,3,4 eV for 3d/4d U=0,2,4,6 eV for 4f/5f
- Initial Magnetic Moments from Neutron-scattering experiments.

Mag-VASP2trace package on BCS (***To be available***)

Only Unitary symmetries Unitary and anti-unitary symmetries

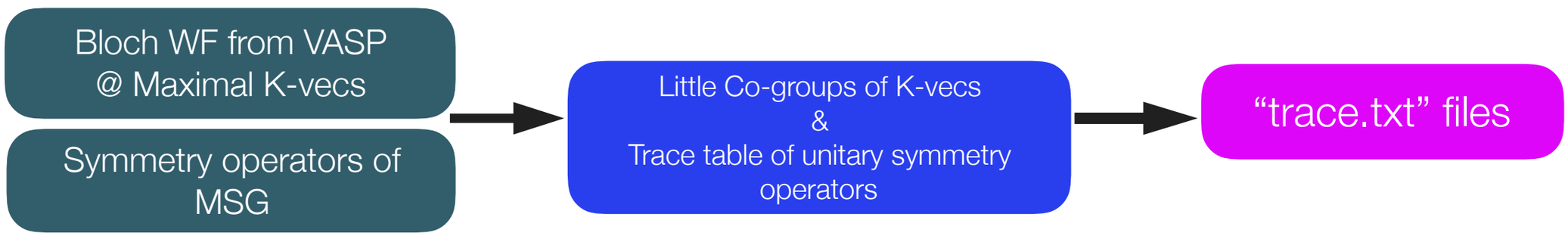
- **Type-I MSG** $M = G$ **Type-II,III,IV MSG** $M = G + H$
- Identify Little co-group G(k) for each Maximal K-vec.

$$\vec{k} = \vec{k} R_j^{-1} + n\vec{g}$$

$$R_j \in G(k)$$

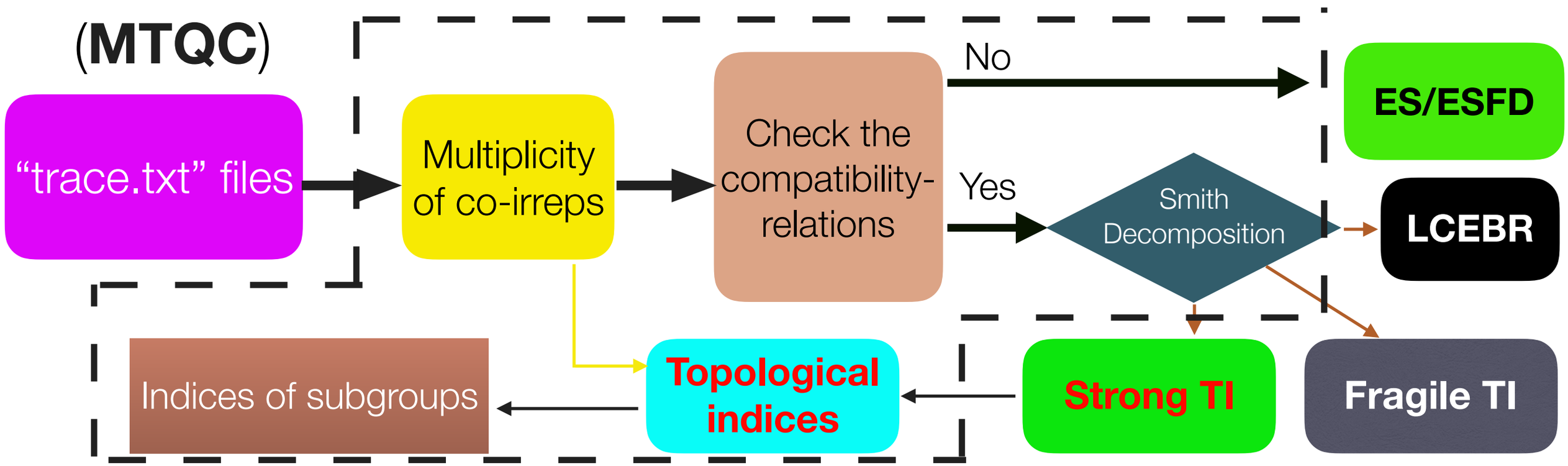
- From Bloch WF $|\Psi_n(k)>$ to symmetry characters

$$< \Psi_n(\vec{k}) | R_{j,\vec{k}} | \Psi_n(\vec{k}) >$$



Calculational methods: New Package 2 Addition to VASP

- **Check MAGMAT Topo.** on BCS (***To be available***)



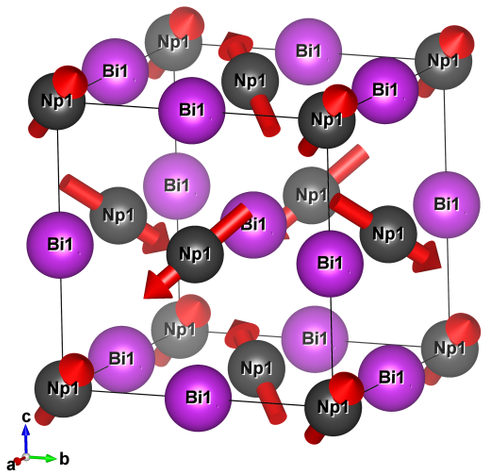
Topological phase diagrams

Self-consistent calculations of 403 of the 549 materials converge
130 materials, 32%, with topological phases at least at one of the U values:

1. 50 most robust topological materials, which maintain the same topology for all U values.
2. 49 of them are topological nontrivial at small U but become trivial as U increases.
3. 20 materials: non-monotonous dependence on U; nontrivial categories at U = 0, different nontrivial categories at finite U.
4. 6 materials are trivial at U = 0, but become topologically nontrivial at some finite U .

Ideal topological materials

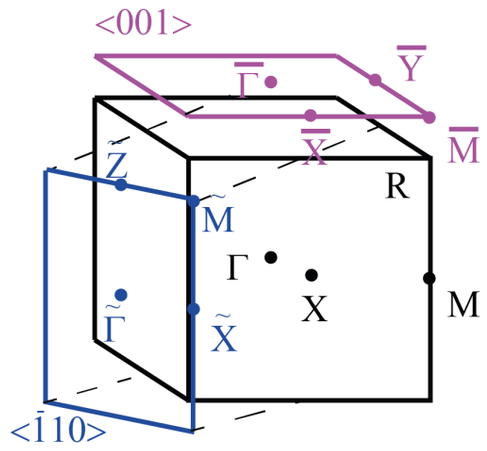
Axion insulator NpBi/NpSb

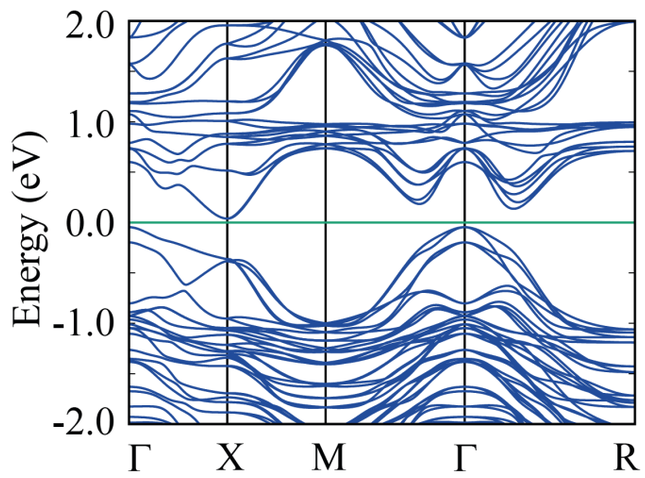


SG: Fm-3m (#225)

MSG: Pn-3m'(#224.113)

T_N=192.5 K





MTQC

Minimal subgroup: $P\bar{1}(No.2.4)$

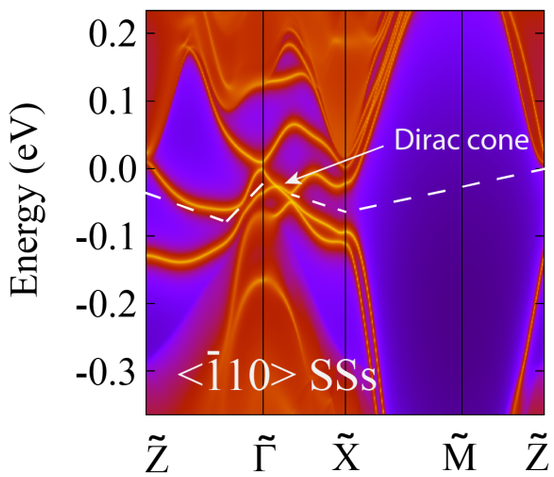
Indice group: $\mathbb{Z}_4 \times \mathbb{Z}_2^3$

$$z_4 = \sum_K n_K^- \ mod\ 4$$

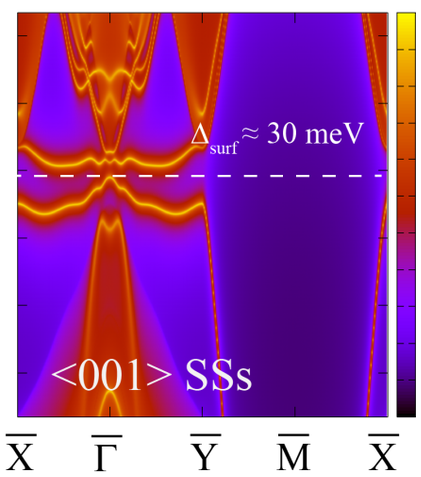
$$z_{2,i=1,2,3} = \sum_{K,K_i=\pi} n_K^- \ mod\ 2$$

$$(z_4, z_{2,1}, z_{2,2}, z_{2,3}) = (2,0,0,0)$$

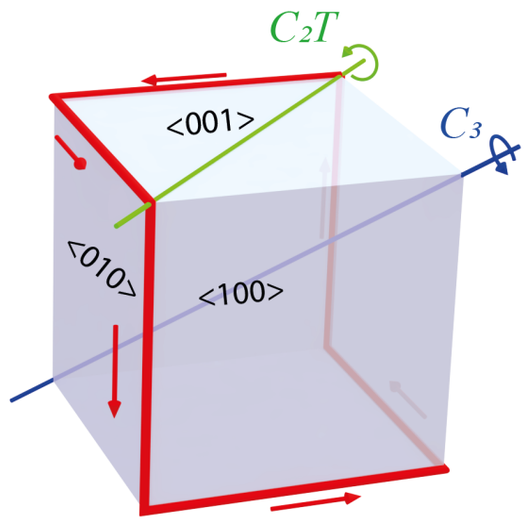
Dirac cone Surface states protected by C2T and Chiral hinge mode



Gapless Surface states protected by C2T



Gapped Surface states



Chiral Hinge mode

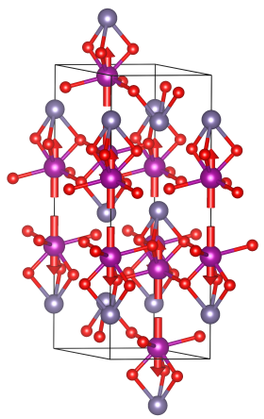
arXiv:1810.02373 (2018) & Phys.Rev.Lett. 122, 256402 (2019)

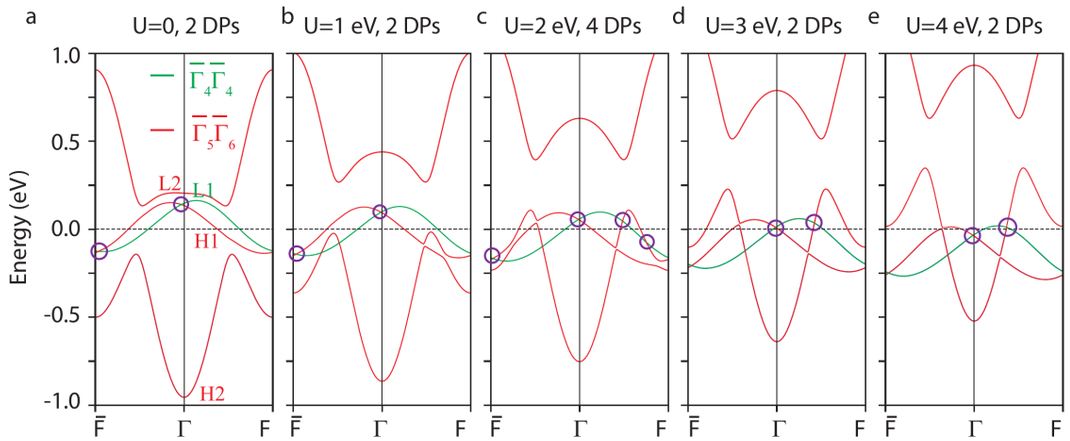
Ideal topological materials

Symmetry enforced Semimetals

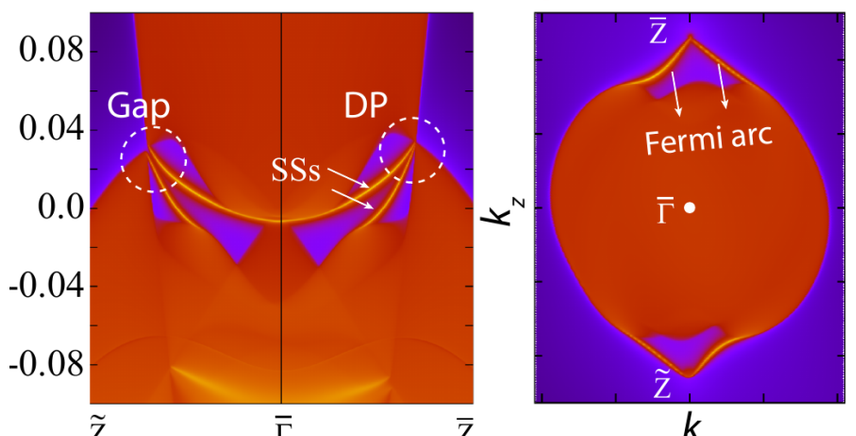
MnGeO3: DSM

Dirac nodes protected by C3z





The two Dirac points are on the C3 axis with different energy.
It doesn't exist in paramagnetic case !!!

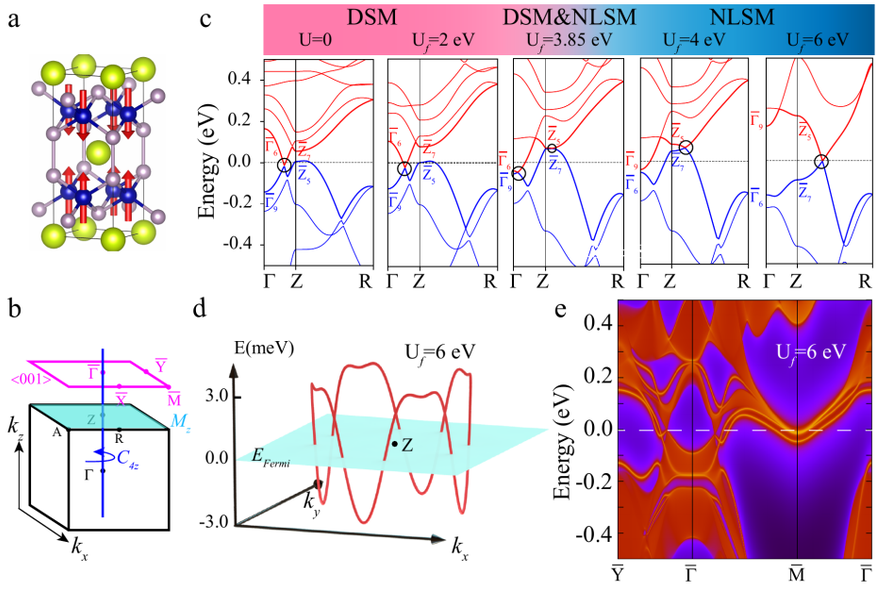


CeCo2P2: HO-DSM/NLSM

Dirac nodes protected by C4z

Nodal-line protected by Mz

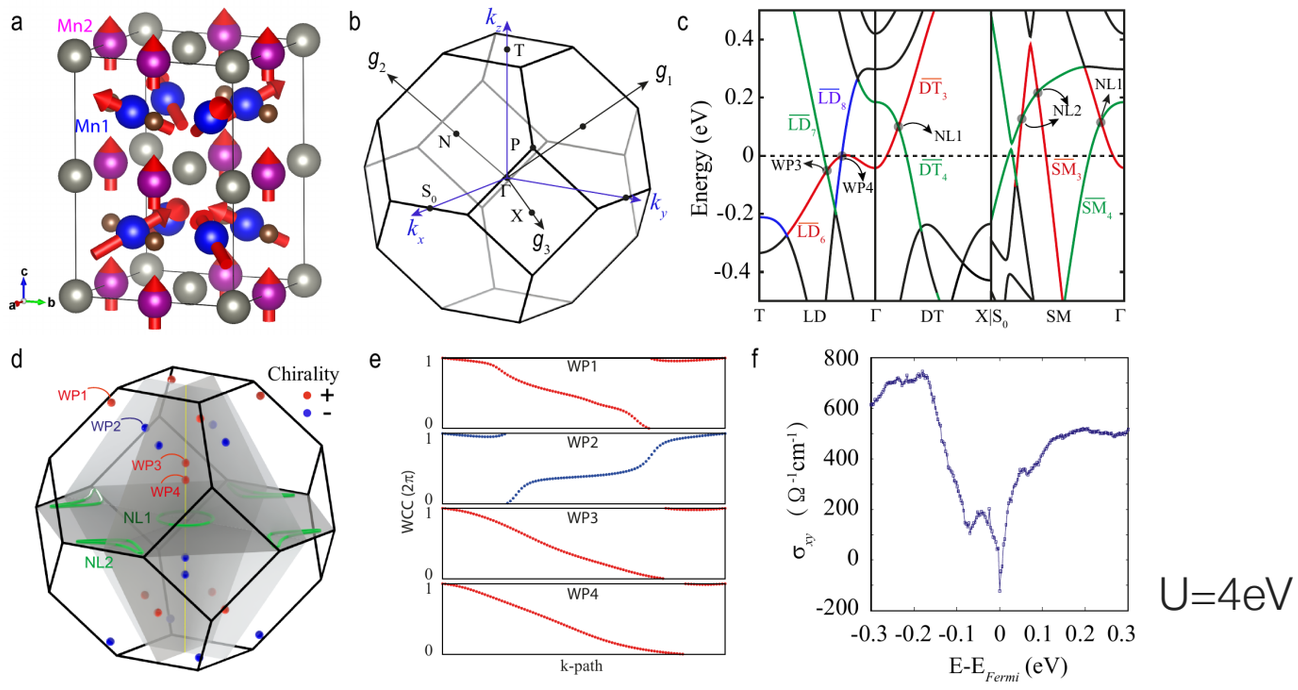
Higher-order SM with co-point group 4mm



Mn3ZnC: WSM/NLSM

Weyl nodes protected by C4z

Nodal-line protected by Mz

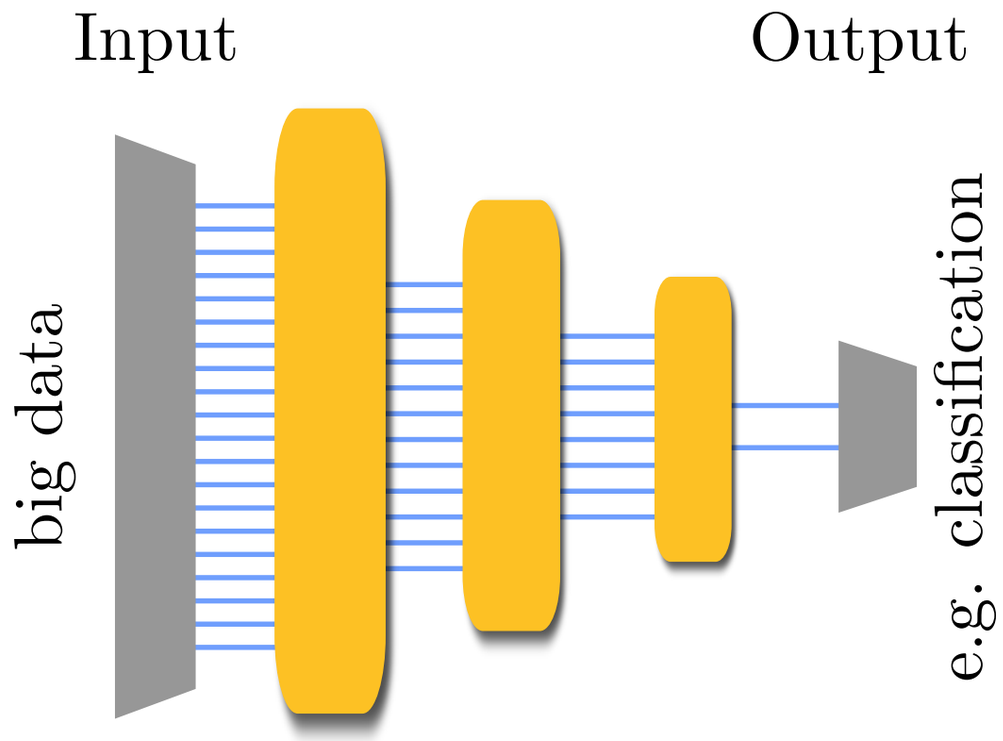


U=4eV

Machine Learning : how to train your network

Supervised learning:

- Train the network with a large amount of labeled data (input-output pairs): Reduce a cost function (distance measure between network output and labels) via e.g. gradient descent.
- Verify the network performance on a distinct test data set.



Unsupervised learning:

Use unlabeled data, the network learns to cluster data/find structure/learn probability distribution of features.

Reinforced learning:

Agents, reward : direct the action of software agents in an environment to maximize some cumulative reward (e.g. videogame score).

Machine Learning Discovery Of Topology Without Band Structure Calculation

Our situation

- **Input:**
  - Nbr of electrons: encoded in binary (easy to detect parity effects, like ESFDs in some specific SGs).
  - Symmetry group: number + frequencies of each class (fingerprint of each SG)
  - Chemical structure: mean number of *s,p,d,f* valence electrons, number of atoms per column/row in the periodic table (to encode chemical similarity).
  - (optional): atom position encoded as average and variance of distances between atoms and their nearest neighbors, coulomb matrix, ...

- **Output:**
  - *Coarse grained label*: Trivial/TI/TSM.
  - Full label: Trivial/NLC/SEBR/ES/ESFD.

- **Training and testing:**
  - 32k materials for the training, 2.5k for the testing.
  - Cross-validation (to estimate the error).

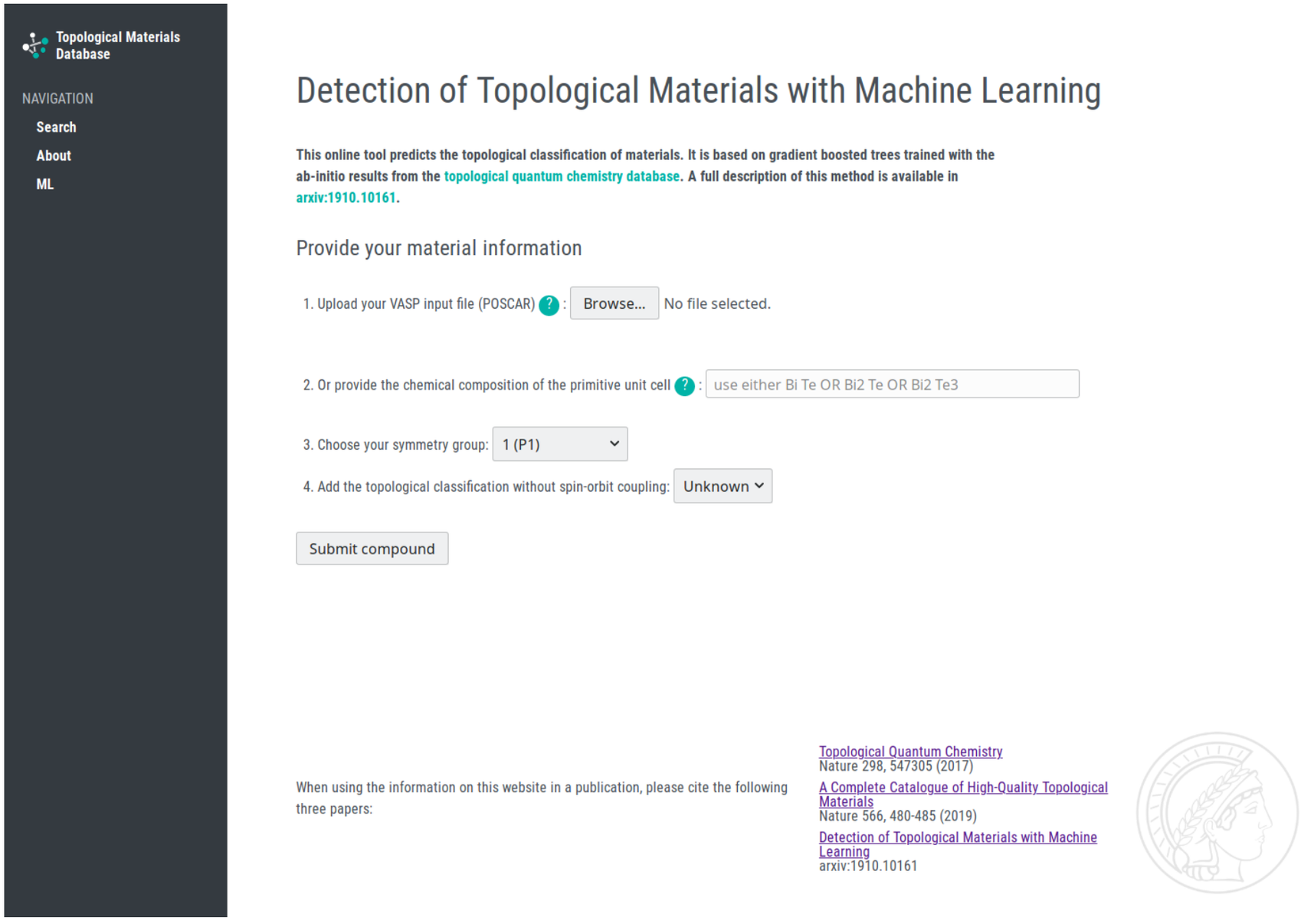
Results: coarse grained label

Model	d	Acc. [%]	F_1 Triv. [%]	F_1 TI [%]	F_1 TSM [%]
Full model (FM)	49	89.7(5)	94.0(3)	70(1)	92.0(5)
FM + Non-SOC	50	92.0(3)	96.5(2)	77(1)	93.3(4)
Baseline model	94	86.0(5)	92.5(5)	67(1)	91.0(5)
spdf+ model	10	87.7(5)	93.0(5)	69(1)	92.0(5)
FM + nearest–neighbor	184	89.0(5)	94.0(3)	69(3)	92.0(5)
FM without SG	48	84.0(5)	91.5(3)	57(2)	86(1)

- d: size of the input vector.
- Full model: SG, N_e, *spdf*+, number of atoms from each periodic table row and column.
- Baseline model: SG, N_e, baseline descriptor (nbr of atoms from each element in stoichiometric formula).

Test your own material

https://www.topologicalquantumchemistry.com/mltqc



Many New Directions:

Phonons

Material Structure Through Topology

Catalysis

Interesting Atomic Insulators

Twisted and Engineered Materials

Interactions

MetaMaterials